Elementary objects of the 1D Hubbard model from its symmetry and exact solution I

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In this first paper of a series of two, we uniquely define the exotic elementary objects that emerge from the interplay of the 1D Hubbard model recently found global $[SU(2) \otimes SU(2) \otimes U(1)]/Z_2^2$ symmetry with the exact Bethe-ansatz (BA) solution. Their occupancy configurations generate the exact energy eigenstates of the model. The results refer to the limit of a very large system in which the thermodynamic BA equations apply. The BA solution choses one of the infinite electron - rotated-electron unitary transformations such that rotated-electron single and double occupancy are a good quantum number for any finite interaction value. This allows a precise operational definition of three exotic elementary objects whose occupancy configurations generate all exact energy eigenstates: spin-less and η-spin-less c fermions, spin-1/2 spinons, and η-spin-1/2 η-spinons. Their occupancy configurations generate as well representations of the c hidden $U(1)$ symmetry, spin $SU(2)$ symmetry, and η-spin $SU(2)$ symmetry algebras, respectively. Furthermore, it is found that the inverse scattering method BA L-matrix and thus the corresponding monodromy matrix are naturally expressed in terms of the seven local generators of the model Hamiltonian electron-interaction term local gauge $SU(2) \otimes SU(2) \otimes U(1)$ symmetry and of the related spin-less and η-spin-less fermion creation and annihilation operators. Our symmetry-related formulation reveals that the M. Takahasi's bound states of *electron n-pairs* described by complex numbers Λ' and his *magnon bound states of n-pairs* described by complex numbers Λ refer to η-spin-singlet configurations involving n anti-bound η-spinon pairs and spin-singlet configurations involving n bound spinon pairs, respectively. In the second paper the scattering theory associated with the present elementary objects is constructed. That study reveals that there is no contradiction whatsoever between the present elementary-object description and those in terms of traditional spinons and holons. The former and the latter are normal ordered relative to the electron vacuum and an initial ground state, respectively. They are found to refer to distinct elementary objects associated with uniquely related scattering-state basis choices. The possibility of such different basis choices stems from the degeneracy of the excited energy eigenstates that span the subspaces of the corresponding scattering theories.

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I. INTRODUCTION

The Hubbard model with nearest-neighbor hopping integral t and on-site repulsion U is possibly the most studied lattice model of correlated electrons. It features electrons that can hop between lattice sites due to the finite hopping integral t. Such sites represent atoms, that are arranged in an ordered, crystalline pattern of well-defined geometry. When two electrons are on the same site, they have to pay the energy U due to their mutual repulsion. This introduces additional electronic correlations beyond those due to the Pauli principle.

On the one-dimensional (1D) lattice the model is exactly solvable. When the number of 1D lattice sites $N_a \gg 1$ is very large the thermodynamic Bethe-ansatz (BA) equations introduced in Ref. [1] apply. The corresponding general BA equations were first derived by the coordinate BA [2]. The same BA equations were later on obtained by use of the alternative algebraic BA inverse-scattering method [3, 4]. The 1D Hubbard model is the simplest condensed-matter toy model for the description of the role of correlations in the exotic properties of quasi-1D materials [5]. It may be realized as well in ultracold atomic 1D optical lattices [6].

The low-energy physics of 1D correlated systems shows universal behavior associated with the so called Luttinger-liquid theory [7]. At finite excitation energy, beyond the linear Luttinger-liquid regime, the separation of the electronic degrees of freedom into exotic different excitation branches prevails. In the case of the 1D Hubbard model, the use of the pseudofermion dynamical theory (PDT) [8–11] revealed that the metallic-phase exponents characterizing their finite-energy correlation function singularities are a function of the excitation momentum and differ signicantly from the predictions of the linear Luttinger-liquid theory [7]. Similar results have been later obtained by a general method applicable to both non-integrable and integrable 1D correlated systems [12–17].

This paper is the first of a series of two [18]. We find that by combining the model global $[SU(2) \otimes SU(2) \otimes U(1)]/Z_2^2$ symmetry [19] with the exact BA solution [1–4], an elementary-object operator formulation emerges where such a global symmetry, which can be rewritten as $[SO(4) \otimes U(1)]/Z_2$, is made explicit. This allows the identification of the

exotic elementary objects whose occupancy configurations generate the model exact energy eigenstates both inside and outside the BA solution and define their operator algebra. The corresponding representation involves seven local operators whose site summation gives the seven generators of the model global symmetry. The local operator whose site summation gives the generator of the global c hidden $U(1)$ symmetry beyond $SO(4)$, is the local density operator of spinless c fermions. The local c fermion operators and the six local operators associated with the spin-1/2 spinon and η-spin-1/2 η-spinon $SU(2)$ algebras that emerge from the symmetry-related representation are mapped from suitable rotated-electron operators by an exact local transformation that does not introduce constraints.

On the other hand, the rotated-electron operators are related to those of the original electrons by a unitary transformation such that rotated-electron double and single site occupancies are good quantum numbers for all finite values of $u = U/4t$. There are infinite such transformations. The interplay of the model global symmetry with its exacts solution determines the unique choice of one of such transformations. From it elementary objects emerge whose occupancy configurations generate the exact energy eigenstates. For large on-site interaction values the η-spin degrees of freedom become unimportant for the low-energy physics and one recovers the usual charge-spin separation. The corresponding charge degrees of freedom refer to the c hidden $U(1)$ symmetry rather than to the $U(1)$ symmetry contained in the η-spin $SU(2)$ symmetry.

The η-spin (and spin) and η-spin projection (and spin projection) of the energy eigenstates are denoted by S_η and $S_\eta^{x_3}$ (and S_s and $S_s^{x_3}$), respectively. The BA solution subspace is spanned either by the lowest-weight states (LWSs) or the highst-weight states (HWSs) of both η-spin and spin algebras, such that $S_\alpha^{x_3} = -S_\alpha$ or $S_\alpha^{x_3} = S_\alpha$, respectively, for $\alpha = c, s$ [20]. We call *Bethe states*, the energy eigenstates inside the BA solution. In this paper we use the LWS representation of that solution. We emphasize that there is no contradiction whatsoever between the global $[SU(2) \otimes SU(2) \otimes U(1)]/Z_2^2 = [SO(4) \otimes U(1)]/Z_2$ symmetry found in Ref. [19] for the Hubbard model on any bipartite lattice and the results of Ref. [20], concerning the counting of the 4^{N_a} energy eigenstates of the Hubbard model in the bipartite 1D lattice. The important point is that it is confirmed in this paper that the BA solution accounts for the quantum number occupancy configurations that generate the representations of the c hidden $U(1)$ symmetry algebra beyond $SO(4)$. Moreover, the energy eigenstates outside the BA solution subspace are found to have exactly the same c hidden $U(1)$ symmetry algebra representations quantum number occupancy configurations as the Bethe states from which they are generated by the off-diagonal η-spin and spin operator algebras.

Although the studies of Ref. [20] have not explicitly considered the model c hidden $U(1)$ symmetry algebra beyond $SO(4)$, they have used the BA solution, which accounts for it. Thus such studies have implicitly accounted for that symmetry, through their counting of the BA solution quantum number occupancy configurations found in this paper to generate the representations of the c hidden $U(1)$ symmetry algebra. Interestingly, that the method of Ref. [20] has counted all 4^{N_a} energy eigenstates gives an exact proof that there are no extra non-Abelian symmetries of the 1D Hubbard model beyond $SO(4) = [SU(2) \otimes SU(2)]/Z_2^2$. This is indeed the case, since the exact additional hidden symmetry found in Ref. [19] is an Abelian $U(1)$ symmetry.

The generator of the new global $U(1)$ symmetry algebra beyond $SO(4)$ is the number of rotated-electron singly occupied sites operator [19], whose eigenvalue we denote by $2S_c$. Alternatively, such a generator can be chosen to be the number of rotated-electron unoccupied and doubly occupied sites operator, whose eigenvalue is $2S_c^h = [N_a - 2S_c]$. The spinon description introduced in this paper is normal-ordered relative to the $S_\eta = N_a/2; S_s = 0; 2S_c = 0$ electron vacuum, in that such a state is not populated by spinons as defined here yet for it the η-spinon number value is maximum and given by N_a. Complementarily, the η-spinon description is normal-ordered relative to the $S_\eta = 0; S_s = 0; 2S_c = N_a$ absolute ground state, since that half-filling and zero-magnetization state is not populated by η-spinons as defined in this paper. For it the spinon number value is maximum and given by N_a. The numbers $2S_c$ and $2S_c^h$ values are also those of c fermions and c fermion holes, respectively, which live on a lattice identical to the original lattice. (Such number values also equal those of the spinons and η-spinons, respectively.) The c fermion, spinon, and η-spinon operator formulation introduced in this paper applies to all electronic-density and spin-density values.

Here and mostly in the second paper, Ref. [18], the relation of the spin-1/2 spinons, η-spin-1/2 η-spinons, and spin-less and η-spin-less c-fermions of the present formulation to other model elementary-object representations is discussed. However, a revision of the vast literature about the model physics description in terms of exotic elementary objects is not among our goals. The elementary object representations of the 1D Hubbard model may be classified into two large groups:

– Elementary-object descriptions normal ordered relative to the electron vacuum, alike the representation in terms of c, $s\nu$, and $c\nu$ pseudoparticles of Refs. [21, 22], which is a generalization of that considered in Refs. [23, 24] for a well-defined model subspace. The elementary-object occupancy configurations of this type of descriptions generate the energy eigenstates from the electron vacuum. The elementary-object operator formulation defined in terms of the original electron operators in this paper belongs to this group of descriptions.

– Elementary-object descriptions normal ordered relative to a well-defined initial ground state. This includes the

traditional spinon and holon descriptions [7, 25–30], which in general share the same spinon definition as spin-1/2 excitations of a $S_s = 0$ ground state. An early example in the literature of spin-1/2 spinons with no charge whose spectrum is associated with a "hole" emerging under a transition from a $S_s = 0$ ground state to an excited state in a sequence of BA spin quantum numbers are the spin-1/2 color spinors introduced for the solvable 1D Gross-Neveu model in Ref. [25]. A similar definition was used in Ref. [26] for the spin-1/2 spin waves of the also BA solvable 1D isotropic Heisenberg antiferromagnetic model. The spin-1/2 spinon description of Refs. [28–30] is a generalization for the 1D Hubbard model of such spin-1/2 color spinors and spin-1/2 spin waves. For the present model such traditional spinon and holon representations are of two types in what the concept of a holon and an antiholon is concerned. For those of which that of Ref. [28] is a representative a holon and an antiholon refers to a "hole" and a "particle", respectively, created in the $k'_j s$ distribution of Ref. [1] under the transition from a $S_s = 0$ ground state of arbitrary electronic density n to an excited state. On the other hand, for the descriptions of which that of Refs. [29, 30] is a representative, a η-spin-1/2 holon and a η-spin-1/2 antiholon is an excitation of the $S_s = S_\eta = 0$ absolute ground state with η-spin projection $+1/2$ and $-1/2$, respectively, associated with a "hole" created in the $k'_j s$ distribution of Ref. [1] under the transition to an excited state. The elementary-object occupancy configurations of this type of descriptions generate the excited energy eigenstates from a well-defined initial ground state.

Our results confirm the validity of the pseudoparticle descriptions of Refs. [21–24]. The relation to the traditional spinon and holon representations [7, 27] is addressed in the second paper. The studies of that paper have selected the results of Refs. [28–30] as a reference. The distinct elementary-object descriptions are found in that paper to follow from different choices of scattering states associated with the dressed S matrices and phase shifts extracted from the BA solution. For all the corresponding scattering theories the asymptotic scattering states must have a well-defined energy. This condition is fulfilled provided that such asymptotic scattering states refer to energy eigenstates of the 1D Hubbard model. As discussed in the second paper, the degeneracy of the excited energy eigenstates of $S_s = 0$ (and $S_\eta = 0$) ground states allows different choices of scattering states and thus of scatterers, scattering centers, and dressed S matrices. Such scatterers and scattering centers are elementary objects whose occupancy configurations refer to the spin (and η-spin and charge) degrees of freedom of the involved excited states. The unitary transformations relating the scattering states of the present elementary-object representation to those of the traditional holons and spinons of the descriptions of Refs. [28] and [29, 30] is studied in the second paper for the 1D Hubbard model in subspaces spanned by excited states of a $S_s = 0$ ground state and the $S_s = S_\eta = 0$ absolute ground state, respectively.

The results of the second paper confirm that there is no contradiction whatsoever between the present elementary-object description and those in terms of traditional spinons and holons as defined in Refs. [28–30]. The corresponding distinct elementary objects refer to different choices of scattering states allowed by the above mentioned degeneracy of the excited energy eigenstates that span the subspaces where the alternative descriptions apply. For instance, the spin-1/2 spinons as defined within the present operator formulation and the descriptions of Refs. [28–30] are found to be completely distinct elementary objects. The elementary objects of Refs. [28] and [29, 30] have been constructed inherently to be excitations of an initial $S_s = 0$ ground state, their number value vanishing for it. In the $u \gg 1$ limit the spin-1/2 spinons of Refs. [28] and [29, 30] in the excited states of the zero-magnetization and half-filled absolute ground state become the spin-1/2 spin-waves of Faddeev and Takhtajan. Those refer to the related 1D spin-1/2 isotropic Heisenberg antiferromagnetic model [26]. On the other hand, within our operator formulation that ground state is populated by $N = N_a$ spin-1/2 spinons, as defined in this paper.

The use of our symmetry-related formulation and corresponding counting of the symmetry $[SU(2) \otimes SU(2) \otimes U(1)]/Z_2^2$ algebra representations in each model subspace with fixed c fermion, spinon, and η-spinon number values provides valuable information on the physical information stored in the occupancy configurations of the BA quantum numbers. For instance, the physical origin of the Takahasi's bound states of *electron n-pairs* described by complex numbers Λ' and his *magnon bound states of n-pairs* described by complex numbers Λ considered in Ref. [1]. We find that they refer to η-spin-singlet configurations involving n anti-bound η-spinon pairs and spin-singlet configurations involving n bound spinon pairs, respectively. The former refer to the η-spin degrees of freedom of n rotated-electron doubly occupied sites and n rotated-electron unoccupied sites. The latter to the spin degrees of freedom of n spin-up rotated-electron singly occupied sites and n spin-down rotated-electron singly occupied sites. The imaginary part of the complex rapidity numbers that emerge in the BA thermodynamic equations of Ref. [1] refers within our operator formulation to the attraction between pre-formed η-spin-neutral η-spinon pairs or spin-neutral spinon pairs.

The studies of this paper account for the model global symmetry and reveal that the former above spin-related $2n$-site rotated-electron occupancies have additional c hidden $U(1)$ symmetry degrees of freedom, which are described by a number $2n$ of c fermions. On the other hand, for those of the latter η-spin-related $2n$-site rotated-electron occupancies such additional degrees of freedom refer to a number $2n$ of c fermion holes. The spin-less c fermions carry electronic charge e and occupy the sites singly occupied by the rotated electrons. They are insensitive to whether such sites are occupied by up-spin or down-spin rotated electrons. That information is stored in the corresponding spin-singlet $2n$-spinon configuration. The c fermion holes refer to the sites doubly occupied or unoccupied by rotated

electrons yet they do not distinguish rotated-electron doubly occupied sites from unoccupied sites. That information is stored in the corresponding η-spin-singlet $2n$-η-spinon configuration. (Since we denote the electron density by n, the Takahashi's pair positive integer numbers n are in the remaining og this paper called ν.)

We are able to access the statistics in terms of the generalized principle of Ref. [31] of the operators associated with the composite 2ν-spinon $s\nu$ objects and 2ν-η-spinon $\eta\nu$ objects in the above spin-singlet and η-spin-singlet configurations, respectively. (Within our notation, $\nu = 1, ..., \infty$ is the number of spinon and η-spinon pairs, respectively.) For each energy eigenstate, the number value of spinons and η-spinons bound and anti-bound, respectively, within such composite objects is fixed. On the other hand, the spinons and η-spinons left over are found to be invariant under the electron - rotated-electron unitary transformation. Those are called in this paper unbound spinons and unbound η-spinons, respectively.

The object representation of Refs. [21, 22] was the starting point of the PDT [8–11]. The operator formulation introduced in this paper is used in the second paper to both confirming the validity of the latter dynamical theory and deepening the understanding of the microscopic scattering processes behind it. Specifically, its studies address the related problem of finding the model natural scatterers and scattering centers. Their dressed S matrix is found to be behind the phase shifts that determine the PDT finite-energy correlation-function exponents momentum and interaction dependence [8–11]. The more recent results of Refs. [12–14, 17] find the same type of behavior in a wider class of 1D correlated systems.

The scattering theory introduced in the second paper is used in its studies to determine the effective charge and spin carried by the elementary objects. The $s\nu$ fermions occupancy configurations are shown to carry the states spin currents whereas the unbounded spinons fully control the effects of the spin transverse fluctuations onto such currents. (The same applies to the effects of the η-spin transverse fluctuations on the charge currents carried by the c fermion and $\eta\nu$ fermion occupancy configurations, which are controlled by the unbounded η-spinon occupancies [32].) Interestingly, due to zero-momentum forward-scattering between the c fermions and $s1$ fermions, for spin densities $m \neq 0$ (and electronic densities $n \neq 1$) the c fermions (and $s1$ fermions) can carry with them spin currents (and charge currents). Such currents are found in the second paper to be determined by the pseudofermion scattering theory phase shifts. On the other hand, the unbound η-spinon and unbound spinon occupancies are found to control the effects of the transverse η-spin and spin fluctuations onto the non-LWSs charge and spin currents, respectively.

The paper is organized as follows: In Section II the 1D Hubbard model is introduced. In addition, our formulation in terms of rotated-electron operators such that single and double occupancy is a good quantum number for $u \neq 0$ is defined. That such rotated-electron description naturally leads to the emergence of three elementary objects whose occupancy configurations generate the exact energy eigenstates is the subject of Section III. In Section IV the three corresponding effective lattices are introduced. The studies of that section also address the consequences of the transformation laws of the η-spinons and spinons under the electron - rotated-electron transformation. The occurrence of hard-core η-spin-neutral composite 2ν-η-spinon-anti-bound bosons and hard-core spin-neutral composite 2ν-spinon-bound objects is confirmed in Section V. The BA quantum numbers are then found to label the $s\nu$ fermions and $\eta\nu$ fermions, respectively. Those are generated from the corresponding hard-core bosons by a Jordan-Wigner transformation. The anti-binding and binding character of the anti-bound η-spinons and bound spinons, respectively, is confirmed. The consequences of the transformation laws of the $s\nu$ fermions and $\eta\nu$ fermions under the electron - rotated-electron transformation, the relation of the simplest excitations to the representations of the model global symmetry algebra, and the properties of the distinct types of elementary objects are issues also addressed in Section V. Section VI is devoted to the study of 1D Hubbard model in physically interesting subspaces. Most of the results of that section focus on the quantum problem described by that model in the subspace with no rotated-electron doubly and unoccupied sites. In the $u \gg 1$ limit no contradiction whatsoever is found between the present spin-1/2 spinon description and the ground-state normal-ordered spin-1/2 wave description of Faddeev and Takhtajan [26]. The concluding remarks are presented in Section VIII. Complementary useful information is provided in three appendices.

II. THE 1D HUBBARD MODEL AND ITS UNIQUELY DEFINED ROTATED-ELECTRON REPRESENTATION

Here we shortly introduce the 1D Hubbard model and its global symmetry found in Ref. [19]. Furthermore, we use the interplay of the model global symmetry with its exact BA solution to define the rotated-electron operators of our formulation.

A. The model and its global symmetry

In a chemical potential μ and magnetic field H the Hubbard Hamiltonian under periodic boundary conditions on a 1D lattice with a site number $N_a \gg 1$ very large and even can be written as,

$$\hat{H} = \hat{H}_{symm} - \sum_{\alpha=\eta,s} \mu_\alpha \, \hat{S}_\alpha^{x_3} \,, \tag{1}$$

where

$$\hat{H}_{symm} \;=\; t\,[\hat{T} + 4u\,\hat{V}_D]\,, \;\; u = U/4t\,; \quad \hat{S}_\eta^{x_3} = -\frac{1}{2}[N_a - \hat{N}]\,; \quad \hat{S}_s^{x_3} = -\frac{1}{2}[\hat{N}_\uparrow - \hat{N}_\downarrow]\,,$$

$$\hat{T} \;=\; -\sum_{\sigma=\uparrow,\downarrow}\sum_{j=1}^{N_a} \left[c_{j,\sigma}^\dagger \, c_{j+1,\sigma} + c_{j+1,\sigma}^\dagger \, c_{j,\sigma}\right] \,; \quad \hat{V}_D = \sum_{j=1}^{N_a} (\hat{n}_{j,\uparrow} - 1/2)\,(\hat{n}_{j,\downarrow} - 1/2) \,. \tag{2}$$

In this equation and throughout this paper de index σ reads $\sigma = \uparrow, \downarrow$ when used as an operator label and $\sigma = +1/2, -1/2$ otherwise, respectively. Moreover, $\hat{T}$ is the kinetic-energy operator in units of t, $\hat{V}_D$ is the electron on-site repulsion operator in units of U, $u = U/4t$ is the electron on-site interaction in units of $4t$, which is often used in this paper, $\mu_c = 2\mu$, $\mu_s = 2\mu_B H$, μ_B is the Bohr magneton, and $\hat{S}_\eta^{x_3}$ and $\hat{S}_s^{x_3}$ are the diagonal generators of the η-spin and spin $SU(2)$ symmetry algebras [33, 34], respectively. The operator $c_{j,\sigma}^\dagger$ (and $c_{j,\sigma}$) that appears in the above equations creates (and annihilates) a spin-projection σ electron at lattice site $j = 1, ..., N_a$. The operator $\hat{n}_{j,\sigma} = c_{j,\sigma}^\dagger \, c_{j,\sigma}$ counts the number of spin-projection σ electrons at such a lattice site. The electronic number operators read $\hat{N} = \sum_{\sigma=\uparrow,\downarrow} \hat{N}_\sigma$ and $\hat{N}_\sigma = \sum_{j=1}^{N_a} \hat{n}_{j,\sigma}$. The momentum operator is given by $\hat{P} = \sum_{\sigma=\uparrow,\downarrow} \sum_k \hat{n}_\sigma(k)\,k$, where the spin-projection σ momentum distribution operator reads $\hat{n}_\sigma(k) = c_{k,\sigma}^\dagger \, c_{k,\sigma}$ and the operator $c_{k,\sigma}^\dagger$ (and $c_{k,\sigma}$) creates (and annihilates) a spin-projection σ electron of momentum k.

In this paper we use in general units of both Planck constant $\hbar$ and lattice constant a one. We denote the electronic charge by e and the lattice length by $L = N_a a = N_a$. The S_α and $S_\alpha^{x_3}$ values of the LWSs and HWSs of the η-spin and spin algebras are such that $S_\alpha = -S_\alpha^{x_3}$ or $S_\alpha = S_\alpha^{x_3}$, respectively. Here $\alpha = \eta$ for η-spin and $\alpha = s$ for spin. The LWSs have electronic densities $n = N/L$ and spin densities $m = [N_\uparrow - N_\downarrow]/L$ obeying the inequalities $0 \le n \le 1$ and $0 \le m \le n$, respectively. The description of the states corresponding to densities such that $0 \le n \le 1$; $1 \le n \le 2$ and $-n \le m \le n$; $-(2-n) \le m \le (2-n)$, respectively, is achieved by application onto the latter states of off-diagonal generators of the η-spin and spin $SU(2)$ symmetry algebras. (The expressions of those are given below in Section II B.) The BA solution refers either to LWSs or HWSs of such algebras. Here we chose the LWS formulation of that solution. Hence for simplicity but without loss in generality, most of our results refer to initial ground states with densities in the ranges defined by the inequalities $0 \le n \le 1$ and $0 \le m \le n$.

An exact result valid for the Hubbard model on any bipartite lattice is that for onsite interaction $u \ne 0$ it has two global $SU(2)$ symmetries [33, 35], which refer to a global $SO(4) = [SU(2) \otimes SU(2)]/Z_2$ symmetry [30, 34]. A recent study of the problem by one of us and collaborators reported in Ref. [19], reveals that an exact extra global c hidden $U(1)$ symmetry emerges for $u \ne 0$, in addition to the $SO(4)$ symmetry. Specifically, the Hubbard model on a bipartite lattice, such as the 1D lattice considered in this paper, has a global $[SU(2) \otimes SU(2) \otimes U(1)]/Z_2^2 = [SO(4) \otimes U(1)]/Z_2 = SO(3) \otimes SO(3) \otimes U(1)$ symmetry. The origin of the global symmetry is a local gauge $SU(2) \otimes SU(2) \otimes U(1)$ symmetry of the model Hamiltonian electron-interaction term first identified in Ref. [36]. That local symmetry becomes for finite U and t a group of permissible unitary transformations. The corresponding local $U(1)$ canonical transformation is not the ordinary gauge $U(1)$ subgroup of electromagnetism. It is rather a "nonlinear" transformation [36].

The electron - rotated-electron unitary transformation plays a key role in the model physics. The global symmetry is closely related to unitary operators $\hat{V} = \hat{V}(u)$ and corresponding rotated-electron operators $\tilde{c}_{j,\sigma} = \hat{V}^\dagger \, c_{j,\sigma} \, \hat{V}$. For those single and double occupancy are good quantum numbers for $u > 0$. The investigations of Ref. [37] reveal that there are infinite unitary transformations and corresponding unitary operators $\hat{V} = \hat{V}(u)$ and choices of rotated electrons. They refer to different choices of the states that span the subspaces with fixed $2S_c$ values. For any of the infinite choices of corresponding unitary operators $\hat{V} = e^{-\hat{S}}$ the following expression refers to the same operator,

$$2\tilde{S}_c \equiv \hat{V}^\dagger \, \hat{Q} \, \hat{V} \,. \tag{3}$$

Here $\hat{Q}$ and the related operator $\hat{D}$ count the number of electron singly-occupied sites and doubly-occupied sites. They read,

$$\hat{Q} = \sum_{j=1}^{N_a} \sum_{\sigma=\uparrow,\downarrow} \hat{n}_{j,\sigma}\,(1 - \hat{n}_{j,-\sigma}) \,; \quad \hat{D} = (\hat{N} - \hat{Q})/2 \,, \tag{4}$$

respectively. The operator provided in Eq. (3) is the above-mentioned global c hidden $U(1)$ symmetry generator whose eigenvalue $2S_c = 0, 1, ...$ is the number of rotated-electron singly occupied sites [19].

B. The specific unitary operator associated with the electron - rotated-electron unitary transformation performed by the exact BA solution

A result of major importance for the present operator formulation is that although addition of chemical-potential and magnetic-field operator terms to the Hubbard model, as given in Eq. (1), lowers its symmetry, such terms commute with it. Therefore, the global symmetry being $SO(3) \otimes SO(3) \otimes U(1)$ implies that the set of independent rotated-electron occupancy configurations that generate the model energy eigenstates generate representations of that global symmetry algebra for all values of the electronic density n and spin density m. Consistent, the number of such independent $[SU(2) \otimes SU(2) \otimes U(1)]/Z_2^2 = SO(3) \otimes SO(3) \otimes U(1)$ symmetry algebra representations equals for the present model its Hilbert-space dimension, 4^{N_a} [19].

The definition of the specific electron - rotated-electron unitary transformation performed by the BA solution is the first step for the introduction of our operator formulation.

1. The Bethe states and corresponding η-spin and spin $SU(2)$ towers of energy eigenstates

It is convenient to express the electron numbers as,

$$
\begin{aligned}
N_\uparrow &= N_\uparrow^0 + n_\eta - n_s; \quad N_\downarrow = N_\downarrow^0 + n_\eta + n_s, \\
N &= N_\uparrow + N_\downarrow = N^0 + 2n_\eta; \quad n_\alpha = S_\alpha + S_\alpha^{x_3} = 0, 1, ..., 2S_\alpha, \quad \alpha = \eta, s.
\end{aligned} \tag{5}
$$

Here $N_\uparrow^0$, $N_\downarrow^0$, and N^0 denotes their values for the Bethe states, which as mentioned in Section I are the energy eigenstates contained in the BA solution subspace,

$$
N_\uparrow^0 = \frac{N_a}{2} - S_\eta + S_s; \quad N_\downarrow^0 = \frac{N_a}{2} - S_\eta - S_s; \quad N^0 = N_a - 2S_\eta. \tag{6}
$$

According to our choice of BA representation, such states are LWSs of both the η-spin and spin algebras, so that for them $n_\eta = n_s = 0$ in Eq. (5). The numbers $n_\eta \geq 0$ and $n_s \geq 0$ given in that equation may be expressed in terms of the η-spin S_η, spin S_s, and general electron numbers of Eq. (5) as,

$$
n_\eta = S_\eta - \frac{1}{2}(N_a - N) = 0, 1, ..., 2S_\eta; \quad n_s = S_s - \frac{1}{2}(N_\uparrow - N_\downarrow) = 0, 1, ..., 2S_s. \tag{7}
$$

The rotated-electron numbers equal those given in Eqs. (5)-(7) for the electrons. In addition, for them single and double occupancy are good quantum numbers, so that the Bethe-state electron numbers of Eq. (6) may be separated into two parts: Those corresponding to the $2S_c$ rotated electrons that singly occupy $2S_c$ sites and to the $[N^0 - 2S_c]$ rotated electrons that doubly occupy $[N^0 - 2S_c]/2$ sites, respectively. Hence for rotated electrons the numbers given in that equation may be rewritten as,

$$
\begin{aligned}
N_\uparrow^0 &= [2S_c + 2S_s]/2 + [N_a - 2S_c - 2S_\eta]/2, \\
N_\downarrow^0 &= [2S_c - 2S_s]/2 + [N_a - 2S_c - 2S_\eta]/2, \\
N^0 &= 2S_c + [N_a - 2S_c - 2S_\eta].
\end{aligned} \tag{8}
$$

Here $[2S_c - 2S_s]/2$ (and $[2S_c + 2S_s]/2$) gives the number of down-spin rotated electrons (and up-spin rotated electrons) that singly occupy sites and $[N_a - 2S_c - 2S_\eta]/2$ is that of down-spin rotated electrons (and up-spin rotated electrons) that doubly occupy sites.

Each site can accommodate two electrons of different spin projection. One can then associate with each site two local orbitals. The number of unoccupied local orbitals, unoccupied spin $\uparrow$ local orbitals, and unoccupied spin $\downarrow$ local orbitals of a Bethe state are conserving numbers given by $N^{h,0} = [2N_a - N^0]$, $N_\uparrow^{h,0} = [N_a - N_\downarrow^0]$, and $N_\downarrow^{h,0} = [N_a - N_\uparrow^0]$, respectively, where the numbers $N_\uparrow^0$, $N_\downarrow^0$, and N^0 are those given in Eq. (8).

Generalization to non-LWSs gives,

$$
\begin{aligned}
N_\uparrow &= N^s_{R,+1/2} + N^\eta_{R,-1/2}, \\
N_\downarrow &= N^s_{R,-1/2} + N^\eta_{R,-1/2}, \\
N^h_\uparrow &= N^s_{R,-1/2} + N^\eta_{R,+1/2}, \\
N^h_\downarrow &= N^s_{R,+1/2} + N^\eta_{R,+1/2}.
\end{aligned}
\tag{9}
$$

Here $N^h_\uparrow = [N_a - N_\downarrow]$, $N^h_\downarrow = [N_a - N_\uparrow]$, and,

$$
\begin{aligned}
N^s_{R,\pm 1/2} &= [2S_c \pm 2S_s \mp 2n_s]/2, \\
N^\eta_{R,\pm 1/2} &= [N_a - 2S_c \pm 2S_\eta \mp 2n_\eta]/2, \\
N^s_R &= [N^s_{R,+1/2} + N^s_{R,-1/2}] = 2S_c, \\
N^\eta_R &= [N^\eta_{R,+1/2} + N^\eta_{R,-1/2}] = [N_a - 2S_c],
\end{aligned}
\tag{10}
$$

are the following rotated-electron site-occupancy numbers,

$$
\begin{aligned}
N^s_{R,+1/2} &\implies \text{Number of spin} \uparrow \text{rotated} - \text{electron singly occupied sites}; \\
N^s_{R,-1/2} &\implies \text{Number of spin} \downarrow \text{rotated} - \text{electron singly occupied sites}; \\
N^\eta_{R,+1/2} &\implies \text{Number of rotated} - \text{electron unoccupied sites}; \\
N^\eta_{R,-1/2} &\implies \text{Number of rotated} - \text{electron doubly occupied sites}; \\
N^s_R &\implies \text{Number of rotated} - \text{electron singly occupied sites}; \\
N^\eta_R &\implies \text{Number of rotated} - \text{electron doubly occupied plus unoccupied sites},
\end{aligned}
\tag{11}
$$

which are good quantum numbers for $u > 0$. We denote the numbers $N^s_{R,\pm 1/2}$ and $N^\eta_{R,\pm 1/2}$ by

$$
\begin{aligned}
N^{s,0}_{R,\pm 1/2} &= [2S_c \pm 2S_s]/2, \\
N^{\eta,0}_{R,\pm 1/2} &= [N_a - 2S_c \pm 2S_\eta]/2,
\end{aligned}
\tag{12}
$$

respectively, for the particular case of the Bethe states for which $n_s = n_\eta = 0$.

Let $\{|\Psi_{l_o,l_\triangle,u}\rangle\}$ be a complete set of 4^{N_a} energy, momentum, η-spin, η-spin projection, spin, and spin-projection eigenstates for $u > 0$. Such states are chosen so that those among them that are LWSs of both the η-spin and spin algebras are the Bethe states. Here $l_\triangle$ is a short notation for the set of four quantum numbers $[2S_c, S_\eta, S_s, n_\eta, n_s]$. The triangle index $\triangle$ in $l_\triangle$ symbolizes the three symmetries: The c hidden $U(1)$ symmetry associated with the number $2S_c$ and the two $SU(2)$ symmetries associated with the numbers S_η, n_η and S_s, n_s, respectively, in $[2S_c, S_\eta, S_s, n_\eta, n_s]$. The index l_o represents all remaining quantum numbers, other than those, that are needed to fully specify an each energy eigenstate $|\Psi_{l_o,l_\triangle,u}\rangle$.

The energy eigenstates of that set that are not contained in the BA solution subspace are generated from the Bethe states as follows,

$$
|\Psi_{l_o,l_\triangle,u}\rangle = \prod_{\alpha=\eta,s} \left[\frac{1}{\sqrt{\mathcal{C}_\alpha}} (\hat{S}^+_\alpha)^{n_\alpha} \right] |\Psi_{l_o,l^0_\triangle,u}\rangle.
\tag{13}
$$

Here,

$$
\begin{aligned}
\mathcal{C}_\alpha &= \langle \Psi_{l_o,l^0_\triangle,u} | (\hat{S}^-_\alpha)^{n_\alpha} (\hat{S}^+_\alpha)^{n_\alpha} | \Psi_{l_o,l^0_\triangle,u} \rangle \\
&= [n_\alpha!] \prod_{j'=1}^{n_\alpha} [2S_\alpha + 1 - j'], \quad n_\alpha = 1, ..., 2S_\alpha, \quad \alpha = \eta, s,
\end{aligned}
\tag{14}
$$

are normalization constants, the η-spin ($\alpha = \eta$) and spin ($\alpha = s$) off-diagonal generators $\hat{S}^+_\alpha$ and $\hat{S}^-_\alpha$ are given below, and $l_\triangle$ and $l^0_\triangle$ stand for $[2S_c, S_\eta, S_s, n_\eta, n_s]$ and $[2S_c, S_\eta, S_s, 0, 0]$, respectively. (Within our notation, $l^0_\triangle$ refers to values of the general index $l_\triangle$ such that $n_\eta = n_s = 0$.)

Analysis of the BA quantum-number occupancy configurations that generate the Bethe states, $|\Psi_{l_o,l^0_\triangle,u}\rangle$, reveals that for $u > 0$ the corresponding wave functions smoothly and continuously behave as a function of u. Hence upon

adiabatically increasing u from any finite value to the $u \to \infty$ limit, each Bethe state, $|\Psi_{l_o,l_{\triangle}^0,u}\rangle$, continuously evolves into a corresponding Bethe state, $|\Psi_{l_o,l_{\triangle}^0,\infty}\rangle$, and vice versa. We emphasize that at $u = \infty$ there are many choices of complete sets of energy eigenstates. Our analysis refers to the specific set of states $\{|\Psi_{l_o,l_{\triangle}^0,\infty}\rangle\}$ generated from the set of finite-u Bethe states $\{|\Psi_{l_o,l_{\triangle}^0,u}\rangle\}$ upon adiabatically increasing u to the $u \to \infty$ limit. There is a unitary transformation connecting the Bethe states $|\Psi_{l_o,l_{\triangle}^0,u}\rangle$ and $|\Psi_{l_o,l_{\triangle}^0,\infty}\rangle$. It is found below that the corresponding unitary operator commutes with the six generators of the two $SU(2)$ symmetries in the model global $[SU(2) \otimes SU(2) \otimes U(1)]/Z_2^2$ symmetry.

2. The electron - rotated-electron unitary operator

Both the corresponding sets of 4^{N_a} states $\{|\Psi_{l_o,l_{\triangle},u}\rangle\}$ for a given fixed $u > 0$ value and $\{|\Psi_{l_o,l_{\triangle},\infty}\rangle\}$, respectively, are complete. The exact BA solution quantum-number independence of u is consistent with the model Hilbert space being the same for all u finite values. Hence it follows from basic quantum-mechanics Hilbert-space and operator properties that for this choice there exists indeed exactly one unitary operator $\hat{V} = \hat{V}(u)$. It is such that any $u \to \infty$ energy eigenstate $|\Psi_{l_o,l_{\triangle},\infty}\rangle$ is transformed onto the corresponding $u > 0$ energy eigenstate $|\Psi_{l_o,l_{\triangle},u}\rangle$ as,

$$|\Psi_{l_o,l_{\triangle},u}\rangle = \hat{V}^{\dagger}|\Psi_{l_o,l_{\triangle},\infty}\rangle \, . \tag{15}$$

The energy eigenstates $|\Psi_{l_o,l_{\triangle},u}\rangle = \hat{V}^{\dagger}|\Psi_{l_o,l_{\triangle},\infty}\rangle$ (one for each value of $u > 0$) that are generated from the same initial $u \to \infty$ energy eingenstate $|\Psi_{l_o,l_{\triangle},\infty}\rangle$ belong to the same V tower. The transformation given in Eq. (15) also relates the Bethe states $|\Psi_{l_o,l_{\triangle}^0,u}\rangle$ to corresponding $u \to \infty$ Bethe states $\{|\Psi_{l_o,l_{\triangle}^0,\infty}\rangle\}$. This is why such a specific unitary transformation is that performed by the exact BA solution.

The corresponding rotated-electron operators are given by,

$$\tilde{c}_{j,\sigma}^{\dagger} = \hat{V}^{\dagger}\,c_{j,\sigma}^{\dagger}\,\hat{V}\,; \quad \tilde{c}_{j,\sigma} = \hat{V}^{\dagger}\,c_{j,\sigma}\,\hat{V}\,; \quad \tilde{n}_{j,\sigma} = \tilde{c}_{j,\sigma}^{\dagger}\,\tilde{c}_{j,\sigma}\,. \tag{16}$$

They are such that rotated-electron single and double occupancy are good quantum numbers for $u > 0$. This follows from the symmetries of the Hamiltonian electron-interaction term. Those are such that all $u \to \infty$ energy eigenstates of the set $\{|\Psi_{l_o,l_{\triangle},\infty}\rangle\}$ are as well eigenstates of the electron single-occupancy operator and double-occupancy operator of Eq. (4). In the $u \to \infty$ limit, the Hilbert space is then classified in subspaces with different numbers of doubly-occupied sites. Each of the states $\{|\Psi_{l_o,l_{\triangle},\infty}\rangle\}$ is contained in only one such subspaces.

The electron and rotated-electron vacuum $|0\rangle$ is invariant under the above unitary transformation. The $u > 0$ energy eigenstates $|\Psi_{l_o,l_{\triangle},u}\rangle = \hat{V}^{\dagger}|\Psi_{l_o,l_{\triangle},\infty}\rangle$ are generated from it by rotated-electron occupancy configurations that are simply obtained from those that generate the corresponding states $|\Psi_{l_o,l_{\triangle},\infty}\rangle = \hat{G}|0\rangle$. The generator onto $|0\rangle$ of the corresponding $u > 0$ energy eigenstates $|\Psi_{l_o,l_{\triangle},u}\rangle = \hat{V}^{\dagger}|\Psi_{l_o,l_{\triangle},\infty}\rangle$ simply reads $\tilde{G} = \hat{V}^{\dagger}\hat{G}\hat{V}$. Such $u > 0$ energy eigenstates may then be written as $|\Psi_{l_o,l_{\triangle},u}\rangle = \tilde{G}|0\rangle$. The rotated-electron occupancy configurations that generate them from the electron and rotated-electron vacuum $|0\rangle$ are the same that generate the corresponding states $|\Psi_{l_o,l_{\triangle},\infty}\rangle = \hat{G}|0\rangle$, provided that electrons are replaced by rotated electrons as defined here. This is why rotated-electron single and double occupancy are good quantum numbers for $u > 0$.

The operational representation of the 1D Hubbard model introduced in this paper refers to the above specific unitary operator and corresponding rotated-electron operators of Eq. (16). As given in that equation, the unitary operator $\hat{V} = \hat{V}(u)$ generates rotated-electron operators from electron operators. We thus call it *electron - rotated-electron unitary operator*. It is associated with one of the infinite unitary transformations considered in Refs. [19, 37]. Except for $u \to \infty$, the rotated electrons emerging from any of such transformations are distinct from the electrons. Given the unitarity character of the transformations associated with the operators $\hat{V} = \hat{V}(U/t)$, they may be used in two different physical problems, which however are mathematically and technically fully equivalent. Those are considered in Refs. [37, 38] and in this paper, respectively.

Specifically, in Refs. [37, 38] it is considered that the rotated creation and annihilation operators of Eq. (16) refer to electrons. Within that choice, except for $u \to \infty$ the Hamiltonian $\hat{V}^{\dagger}\hat{H}_{symm}\hat{V}^{\dagger}$ obtained by rotating the Hamiltonian $\hat{H}_{symm}$ of Eq. (2) is not the Hubbard model. Instead, it is a *rotated Hubbard Hamiltonian* of a model for which electron double occupancy and single occupancy are good quantum numbers. On the other hand, within the alternative physical problem studied here, the rotated creation and annihilation operators of Eq. (16) refer to *rotated electrons*, which for finite u values are objects distinct from the electrons. Within it the Hamiltonian $\hat{V}^{\dagger}\hat{H}_{symm}\hat{V}^{\dagger}$ is the Hubbard model expressed in terms of rotated-electron creation and annihilation operators. For that problem rotated-electron double occupancy and single occupancy are good quantum numbers for $u > 0$.

We associate with any operator $\hat{O}$ an operator $\tilde{O} = \hat{V}^\dagger \hat{O} \hat{V}$. It has the same expression in terms of rotated-electron creation and annihilation operators as $\hat{O}$ in terms of electron creation and annihilation operators, respectively. Our convention is that marks placed over letters being a caret or a tilde denote operators. (A first exception are the electron operators of Eq. (16), which we denote by $c^\dagger_{j,\sigma}$ and $c_{j,\sigma}$ rather than by $\hat{c}^\dagger_{j,\sigma}$ and $\hat{c}_{j,\sigma}$, respectively.)

The unitary operator $\hat{V}$ of our formulation is uniquely defined by its $4^{N_a} \times 4^{N_a}$ matrix elements, $\langle \Psi_{l_o,l_\triangle,u}|\hat{V}|\Psi_{l',l'_\triangle,u}\rangle$. That, as justified below, for $u > 0$ the unitary operator $\hat{V} = \hat{V}(u)$ commutes with the six generators of the global η-spin and spin $SU(2)$ symmetries, implies that the matrix elements between energy eigenstates with different values of S_η, S_s, n_η, and n_s and thus of $l_\triangle$ vanish. Hence the finite matrix elements are between states with the same $l_\triangle$ values. We denote them by V_{l_o,l'_o},

$$
\begin{aligned}
V_{l_o,l'_o} &= \langle \Psi_{l_o,l_\triangle,u}|\hat{V}|\Psi_{l',l_\triangle,u}\rangle = \langle \Psi_{l',l_\triangle,\infty}|\hat{V}^\dagger|\Psi_{l_o,l_\triangle,\infty}\rangle^* \\
&= \langle \Psi_{l_o,l_\triangle,u}|\Psi_{l',l_\triangle,\infty}\rangle = \langle \Psi_{l',l_\triangle,\infty}|\Psi_{l_o,l_\triangle,u}\rangle^*.
\end{aligned}
\tag{17}
$$

For $u \to \infty$ rotated electrons become electrons, so that the matrix representing the unitary operator $\hat{V}$ becomes the $4^{N_a} \times 4^{N_a}$ unit matrix whose entries read $\langle \Psi_{l_o,l_\triangle,\infty}|\hat{V}|\Psi_{l',l'_\triangle,\infty}\rangle = \delta_{l_o,l'_o}\delta_{l_\triangle,l'_\triangle}$. Here and throughout this paper δ_{l_o,l'_o} and $\delta_{l_\triangle,l'_\triangle}$ are the usual Kronecker symbols.

In the following we define the electron - rotated-electron unitary operator $\hat{V}$ by expressing all its finite matrix elements V_{l_o,l'_o} in terms of known amplitudes of the exact BA solution.

3. The unitary-operator matrix elements between Bethe states

We start by considering the matrix elements of the specific electron - rotated-electron unitary operator considered here between Bethe states. Let $|x_1, ..., x_{N^0}; y_1, ..., y_{N^0_\downarrow}\rangle$ denote the state in which the N^0 electrons are located at sites of spatial coordinates $x_1, ..., x_{N^0}$ and the $N^0_\downarrow$ down-spin electrons among those are at sites of spatial coordinates $y_1, ..., y_{N^0_\downarrow}$. Consistent with the numbers given in Eqs. (8) and (12), let $|u; x^s_1, ..., x^s_{N^s_R}; x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}; x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}}\rangle$ denote the state in which a number $N^{s,0}_R = 2S_c$ of rotated electrons singly occupy sites of spatial coordinates $x^s_1, ..., x^s_{N^{s,0}_R}$, a number $N^{\eta,0}_{R,-1/2} = [N_a - 2S_c - 2S_\eta]/2$ of rotated electrons doubly occupy sites of spatial coordinates $x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}$, and a number $N^{s,0}_{R,-1/2} = [2S_c - 2S_s]/2$ of spin-down rotated electrons singly occupy sites of spatial coordinates $x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}}$. The relation of the rotated-electron operators to the electron operators is a function of u. Thus the expression of the states $|u; x^s_1, ..., x^s_{N^s_R}; x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}; x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}}\rangle$ in terms of the above N^0electron states is u dependent. Furthermore, the sets of states $\{|u; x^s_1, ..., x^s_{N^s_R}; x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}; x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}}\rangle\}$ are different for different u values. Only at a fixed u value are such states orthogonal. (Since as $u \to \infty$ rotated electrons become electrons, one has that $|\infty; x^s_1, ..., x^s_{N^s_R}; x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}; x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}}\rangle$ and $|x_1, ..., x_{N^0}; y_1, ..., y_{N^0_\downarrow}\rangle$ are two alternative notations for the same state.)

The above energy eigenstates may be written in two alternative representations as,

$$
\begin{aligned}
|\Psi_{l_o,l^0_\triangle,u}\rangle &= \sum_{1 \le x_i \le N_a} f_{l_o,l^0_\triangle,u}(x_1, ..., x_{N^0}; y_1, ..., y_{N^0_\downarrow})|x_1, ..., x_{N^0}; y_1, ..., y_{N^0_\downarrow}\rangle, \\
&= \sum_{1 \le x_i \le N_a} f_{l_o,l^0_\triangle,rt}(x^s_1, ..., x^s_{N^s_R}; x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}; x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}}) \\
&\quad \times |u; x^s_1, ..., x^s_{N^s_R}; x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}; x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}}\rangle,
\end{aligned}
\tag{18}
$$

respectively. In both cases the summation is over all $x_1, ..., x_{N^0}$ from 1 to N_a. For $u > 0$ the quantity $f_{l_o,l^0_\triangle,u}$ is the amplitude of the state $|x_1, ..., x_{N^0}; y_1, ..., y_{N^0_\downarrow}\rangle$ and $f_{l_o,l^0_\triangle,rt}$ that of the state

$$|u; x_1^s, ..., x_{N_R^s}^s; x_1^d, ..., x_{N_{R,-1/2}^{\eta,0}}^d; x_1^{s\downarrow}, ..., x_{N_{R,-1/2}^{s,0}}^{s\downarrow}\rangle,$$

$$f_{l_o, l_\triangle^0, u}(x_1, ..., x_{N^0}; y_1, ..., y_{N_\downarrow^0}) = \langle x_1, ..., x_{N^0}; y_1, ..., y_{N_\downarrow^0}|\Psi_{l_o, l_\triangle^0, u}\rangle,$$

$$f_{l_o, l_\triangle^0, rt}(x_1^s, ..., x_{N_R^s}^s; x_1^d, ..., x_{N_{R,-1/2}^{\eta,0}}^d; x_1^{s\downarrow}, ..., x_{N_{R,-1/2}^{s,0}}^{s\downarrow}) =$$

$$\langle u; x_1^s, ..., x_{N_R^s}^s; x_1^d, ..., x_{N_{R,-1/2}^{\eta,0}}^d; x_1^{s\downarrow}, ..., x_{N_{R,-1/2}^{s,0}}^{s\downarrow}|\Psi_{l_o, l_\triangle^0, u}\rangle. \tag{19}$$

By using the first of the state expressions provided in Eq. (18) in the matrix elements general expression of Eq. (17), those may be rewritten as,

$$V_{l_o, l_o'} = \langle \Psi_{l_o, l_\triangle^0, u}|\hat{V}|\Psi_{l', l_\triangle^0, u}\rangle = \langle \Psi_{l_o, l_\triangle^0, u}|\Psi_{l', l_\triangle^0, \infty}\rangle$$

$$= \sum_{1 \le x_i \le N_a} f_{l_o, l_\triangle^0, u}^*(x_1, ..., x_{N^0}; y_1, ..., y_{N_\downarrow^0}) f_{l', l_\triangle^0, \infty}(x_1, ..., x_{N^0}; y_1, ..., y_{N_\downarrow^0}). \tag{20}$$

To arrive to this expression, we have used the orthonormality of the states $|x_1, ..., x_{N^0}; y_1, ..., y_{N_\downarrow^0}\rangle$.

For $u > 0$ the state $|\Psi_{l_o, l_\triangle^0, u}\rangle$ is an energy eigenstate and the electron and the $S_\eta = N_a/2; S_s = 0; 2S_c = 0$ rotated-electron vacuum $|0\rangle$ is invariant under $\hat{V}$. It follows that $\hat{V}|0\rangle = |0\rangle$ and thus $\langle 0|\hat{V}^\dagger = \langle 0|$. That combined with the unitarity of $\hat{V}$ reveals that the amplitude $f_{l_o, l_\triangle^0, rt}(x_1^s, ..., x_{N_R^s}^s; x_1^d, ..., x_{N_{R,-1/2}^{\eta,0}}^d; x_1^{s\downarrow}, ..., x_{N_{R,-1/2}^{s,0}}^{s\downarrow})$ given by $\langle u; x_1^s, ..., x_{N_R^s}^s; x_1^d, ..., x_{N_{R,-1/2}^{\eta,0}}^d; x_1^{s\downarrow}, ..., x_{N_{R,-1/2}^{s,0}}^{s\downarrow}|\Psi_{l_o, l_\triangle^0, u}\rangle$ equals the amplitude $f_{l_o, l_\triangle^0, \infty}(x_1, ..., x_{N^0}; y_1, ..., y_{N_\downarrow^0}) = \langle x_1, ..., x_{N^0}; y_1, ..., y_{N_\downarrow^0}|\Psi_{l_o, l_\triangle^0, \infty}\rangle$, yet refers to a different notation. Indeed,

$$f_{l_o, l_\triangle^0, rt}(x_1^s, ..., x_{N_R^s}^s; x_1^d, ..., x_{N_{R,-1/2}^{\eta,0}}^d; x_1^{s\downarrow}, ..., x_{N_{R,-1/2}^{s,0}}^{s\downarrow}) = \langle u; x_1^s, ..., x_{N_R^s}^s; x_1^d, ..., x_{N_{R,-1/2}^{\eta,0}}^d; x_1^{s\downarrow}, ..., x_{N_{R,-1/2}^{s,0}}^{s\downarrow}|\Psi_{l_o, l_\triangle^0, u}\rangle$$

$$= \langle 0|[\tilde{c}_{1,\sigma_1}\tilde{c}_{2,\sigma_2}...\tilde{c}_{N^0,\sigma_{N^0}}]|\Psi_{l_o, l_\triangle^0, u}\rangle$$

$$= \langle 0|[\hat{V}^\dagger c_{1,\sigma_1}\hat{V}\hat{V}^\dagger c_{2,\sigma_2}\hat{V}...\hat{V}^\dagger c_{N^0,\sigma_{N^0}}\hat{V}]\hat{V}^\dagger|\Psi_{l_o, l_\triangle^0, \infty}\rangle$$

$$= \langle 0|c_{1,\sigma_1}c_{2,\sigma_2}...c_{N^0,\sigma_{N^0}}|\Psi_{l_o, l_\triangle^0, \infty}\rangle$$

$$= \langle x_1, ..., x_{N^0}|\Psi_{l_o, l_\triangle^0, \infty}\rangle$$

$$= f_{l_o, l_\triangle^0, \infty}(x_1, ..., x_{N^0}; y_1, ..., y_{N_\downarrow^0}). \tag{21}$$

Here both the relations $|\Psi_{l_o, l_\triangle^0, u}\rangle = \hat{V}^\dagger|\Psi_{l_o, l_\triangle^0, \infty}\rangle$ of Eq. (15), which is also valid for Bethe states, and $\tilde{c}_{j,\sigma} = \hat{V}^\dagger c_{j,\sigma}\hat{V}$ of Eq. (16) were used.

From the above results one finds that for $u > 0$ and the rotated electrons generated from the electrons by the electron - rotated-electron unitary operator $\hat{V}$ as defined in this paper the amplitude $f_{l_o, l_\triangle^0, rt}$ is independent of u. This is due to an exact compensation of the u dependences of the states $|\Psi_{l_o, l_\triangle^0, u}\rangle$ and $|u; x_1^s, ..., x_{N_R^s}^s; x_1^d, ..., x_{N_{R,-1/2}^{\eta,0}}^d; x_1^{s\downarrow}, ..., x_{N_{R,-1/2}^{s,0}}^{s\downarrow}\rangle$, respectively. Specifically, by combining the following relation between the N^0electron amplitude $f_{l_o, l_\triangle^0, u}(x_1, ..., x_{N^0}; y_1, ..., y_{N_\downarrow^0})$ and N^0-rotated-electron amplitude $f_{l_o, l_\triangle^0, rt}(x_1^s, ..., x_{N_R^s}^s; x_1^d, ..., x_{N_{R,-1/2}^{\eta,0}}^d; x_1^{s\downarrow}, ..., x_{N_{R,-1/2}^{s,0}}^{s\downarrow})$,

$$f_{l_o, l_\triangle^0, u}(x_1, ..., x_{N^0}; y_1, ..., y_{N_\downarrow^0}) = \sum_{1 \le x_i' \le N_a} f_{l_o, l_\triangle^0, rt}(x_1^{s'}, ..., x_{N_R^s}^{s}{}'; x_1^{d'}, ..., x_{N_{R,-1/2}^{\eta,0}}^{d}{}'; x_1^{s\downarrow'}, ..., x_{N_{R,-1/2}^{s,0}}^{s\downarrow}{}')$$

$$\times \langle x_1, ..., x_{N^0}; y_1, ..., y_{N_\downarrow^0}|rt; x_1^{s'}, ..., x_{N_R^s}^{s}{}'; x_1^{d'}, ..., x_{N_{R,-1/2}^{\eta,0}}^{d}{}'; x_1^{s\downarrow'}, ..., x_{N_{R,-1/2}^{s,0}}^{s\downarrow}{}'\rangle, \tag{22}$$

with the u independence of $f_{l_o, l_\triangle^0, rt}(x_1^s, ..., x_{N_R^s}^s; x_1^d, ..., x_{N_{R,-1/2}^{\eta,0}}^d; x_1^{s\downarrow}, ..., x_{N_{R,-1/2}^{s,0}}^{s\downarrow})$, one finds,

$$\frac{\partial}{\partial u} f_{l_o, l_\triangle^0, u}(x_1, ..., x_{N^0}; y_1, ..., y_{N_\downarrow^0}) =$$

$$\sum_{1 \le x_i' \le N_a} f_{l_o, l_\triangle^0, rt}(x_1^{s'}, ..., x_{N_R^s}^{s}{}'; x_1^{d'}, ..., x_{N_{R,-1/2}^{\eta,0}}^{d}{}'; x_1^{s\downarrow'}, ..., x_{N_{R,-1/2}^{s,0}}^{s\downarrow}{}')$$

$$\times \frac{\partial}{\partial u} \langle x_1, ..., x_{N^0}; y_1, ..., y_{N_\downarrow^0}|rt; x_1^{s'}, ..., x_{N_R^s}^{s}{}'; x_1^{d'}, ..., x_{N_{R,-1/2}^{\eta,0}}^{d}{}'; x_1^{s\downarrow'}, ..., x_{N_{R,-1/2}^{s,0}}^{s\downarrow}{}'\rangle. \tag{23}$$

By use of both the second state expression provided in Eq. (18) and the amplitude relation of Eq. (21) in the matrix elements general expression of Eq. (17) those may, alternatively to their expression given in Eq. (20), be written in terms of rotated-electron amplitudes as follows,

$$
\begin{aligned}
V_{l_o,l'_o} &= \sum_{1 \le x_i \le N_a} \sum_{1 \le x'_i \le N_a} f^*_{l_o,l^0_\triangle,rt}(x^s_1, ..., x^s_{N^s_R}; x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}; x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}}) \\
&\times f_{l',l^0_\triangle,rt}(x^{s\,'}_1, ..., x^{s}_{N^s_R}{}', x^{d\,'}_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}{}'; x^{s\downarrow\,'}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}}{}') \\
&\times \langle u; x^s_1, ..., x^s_{N^s_R}; x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}; x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}} | \infty; x^{s\,'}_1, ..., x^s_{N^s_R}{}'; x^{d\,'}_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}{}'; x^{s\downarrow\,'}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}}{}' \rangle. \quad (24)
\end{aligned}
$$

Hence the whole u dependence of this V_{l_o,l'_o} expression is in the state-product factor $\langle u; x^s_1, ..., x^s_{N^s_R}; x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}; x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}} | \infty; x^{s\,'}_1, ..., x^s_{N^s_R}{}'; x^{d\,'}_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}{}'; x^{s\downarrow\,'}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}}{}' \rangle$.

We proceed by expressing the matrix elements of the electron - rotated-electron unitary operator provided in Eqs. (20) and (24), which are a particular case of those given in Eq. (17), in terms of known quantities of the exact BA solution. This requires the expression of the amplitudes of Eq. (19) in terms of such quantities.

The amplitude $f_{l_o,l^0_\triangle,u}(x_1, ..., x_{N^0}; y_1, ..., y_{N^0_\downarrow})$ appearing in the matrix elements provided in Eq. (20) has been calculated by use of the exact BA solution [39]. Here we write it as,

$$
\begin{aligned}
f_{l_o,l^0_\triangle,u}(x_1, ..., x_{N^0}; y_1, ..., y_{N^0_\downarrow}) &= \mathcal{C}_u[g_P(x_1, ..., x_{N^0}) \times g^\downarrow_P(y_1, ..., y_{N^0_\downarrow})], \\
g_P(x_1, ..., x_{N^0}) &= \sum_P (-1)^Q (-1)^P e^{i \sum_{j=1}^{N^0} k_{Pj} x_{Qj}}, \\
\mathcal{C}_u &= \frac{1}{\sqrt{\sum_{1 \le x_i \le N_a} |g_P(x_1, ..., x_{N^0}) g^\downarrow_P(y_1, ..., y_{N^0_\downarrow})|^2}},
\end{aligned} \quad (25)
$$

where the permutation Q is defined by the inequality,

$$
1 \le x_{Q1} \le x_{Q2} \le ... \le x_{QN^0} \le N_a. \quad (26)
$$

The $\sum_P$ summation runs over all permutations P of the BA quantum numbers k_{Pj} considered in Refs. [39] and [40]. The function $g^\downarrow_P(y_1, ..., y_{N^0_\downarrow})$ in Eq. (25) obeys the equality,

$$
g^\downarrow_P(y_1, ..., y_{N^0_\downarrow}) = \varphi_P(\sigma_{Q1}, \sigma_{Q2}, ..., \sigma_{QN^0}), \quad (27)
$$

where $\varphi_P(\sigma_{Q1}, \sigma_{Q2}, ..., \sigma_{QN^0})$ is defined in Eqs. (2.7) - (2.10) of Ref. [39]. Our notation for it, $g^\downarrow_P(y_1, ..., y_{N^0_\downarrow})$, follows from that function only depending explicitly on the spatial coordinates $y_1, ..., y_{N^0_\downarrow}$ of the down spins in the series $\sigma_{Q1}, \sigma_{Q2}, ..., \sigma_{QN^0}$, in increasing order,

$$
1 \le y_1 < y_2 < ... < y_{N^0_\downarrow} \le N^0. \quad (28)
$$

We profit now from the equality $f_{l_o,l^0_\triangle,rt} = f_{l_o,l^0_\triangle,\infty}$ of Eq. (21) to express the amplitude $f_{l_o,l^0_\triangle,rt}(x^s_1, ..., x^s_{N^s_R}; x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}; x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}})$ in the matrix elements expression provided in Eq. (24) in terms of known quantities of the exact BA solution. In the $u \to \infty$ limit, the related amplitude $f_{l_o,l^0_\triangle,\infty}$ has a simpler form, first given in Eq. (2.23) of Ref. [40]. Combination of the results of that reference with the properties of the electron - rotated-electron unitary transformation confirms that $f_{l_o,l^0_\triangle,rt}$ is a function of the rotated-electron singly occupied sites of spatial coordinates $x^s_1, ..., x^s_{N^s_R}$, rotated-electron doubly occupied sites of spatial coordinates $x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}$, and spin-down rotated-electron singly occupied sites of spatial coordinates $x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}}$. For $u > 0$ this u-independent amplitude reads,

$$
\begin{aligned}
&f_{l_o,l^0_\triangle,rt}(x^s_1, ..., x^s_{N^s_R}; x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}; x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}}) = \\
&\mathcal{C}_{rt}[\phi^c_{U(1)}(x^s_1, ..., x^s_{N^s_R}) \times \phi^\eta_{SU(2)}(x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}) \times \phi^s_{SU(2)}(x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}})],
\end{aligned} \quad (29)
$$

where,

$$\phi^c_{U(1)}(x^s_1, ..., x^s_{N^s_R}) = (-1)^Q \left[\sum_P (-1)^P e^{i \sum_{j=1}^{2S_c} k_{Pj} x^s_{Qj}} \right] = (-1)^Q \det \left[e^{ik_{Pj} x^s_{Qj}} \right],$$

$$\phi^\eta_{SU(2)}(x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}) = (-1)^{[N^0 - 2S_c]/2} \phi_1(x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}),$$

$$\phi^s_{SU(2)}(x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}}) = \phi_2(x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}}), \tag{30}$$

and

$$\mathcal{C}_{rt} = \frac{1}{\sqrt{\sum_{1 \leq x_i \leq N_a} |\phi^c_{U(1)}(x^s_1, ..., x^s_{N^s_R}) \, \phi^\eta_{SU(2)}(x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}) \, \phi^s_{SU(2)}(x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}})|^2}}, \tag{31}$$

is a normalization constant. An important property is that the amplitude of Eq. (29) factorizes into the three functions $\phi^c_{U(1)}(x^s_1, ..., x^s_{N^s_R})$, $\phi_1(x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}})$, and $\phi_2(x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}})$ associated with the c hidden $U(1)$ symmetry, η-spin $SU(2)$ symmetry, and spin $SU(2)$ symmetry, respectively.

Concerning the function $\phi^c_{U(1)}(x^s_1, ..., x^s_{N^s_R})$, the permutation Q appearing in the expression of Eq. (30) arranges the spatial coordinates $x^s_1, ..., x^s_{N^s_R}$ into non-decreasing order with the restriction that from two equal coordinates that of the rotated electron with down spin must come first. The spatial coordinates $x^s_1, ..., x^s_{N^s_R}$ refer to the rotated-electron singly occupied sites in the original lattice. The coordinates $x^d_1, ..., x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}$ correspond to the doubly occupied sites in an effective lattice containing only the doubly and unoccupied sites. The spatial coordinates $x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}}$ refer to the down spins in increasing order in an effective lattice containing only singly occupied sites. The determinant in that function expression depends only on the spatial coordinates of the $2S_c$ sites singly occupied by the rotated electrons and not on their spins, $\sigma_{Q1}, \sigma_{Q2}, ..., \sigma_{Q2S_c}$.

Concerning the functions $\phi_1(x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}})$ and $\phi_2(x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}})$, for simplicity we omit here their expressions. Indeed, they have exactly the same form as those appearing in the $u \to \infty$ limit in the wavefunction for electrons. Such functions are given in Ref. [40]. (Specifically, see Eq. (2.24) of that reference for $u \gg 1$ plus the text in the paragraph just after that equation.) They are such that the corresponding functions $\phi^\eta_{SU(2)} = (-1)^{[N^0 - 2S_c]/2} \phi_1$ and $\phi^s_{SU(2)} = \phi_2$ have the following limiting behaviors,

$$\phi^\eta_{SU(2)} = 1 \text{ for } N^\eta_R = [N_a - 2S_c] = 2S_\eta; \quad \phi^s_{SU(2)} = 1 \text{ for } N^s_R = 2S_c = 2S_s. \tag{32}$$

In spite of the exact mathematical equality $f_{l_o, l^0_\triangle, rt} = f_{l_o, l^0_\triangle, \infty}$, the amplitudes $f_{l_o, l^0_\triangle, rt}$ and $f_{l_o, l^0_\triangle, \infty}$ have different physical meanings. On the one hand, the amplitude $f_{l_o, l^0_\triangle, rt}$ and the above rotated-electron spatial coordinates $x^s_1, ..., x^s_{N^s_R}, x^d_1, ..., x^d_1, ..., x^d_{N^{\eta,0}_{R,-1/2}}$, and $x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}}$ on which it depends are valid for the whole $u > 0$ range. On the other hand, the value of the amplitude $f_{l_o, l^0_\triangle, \infty}$ is mathematically identical to that provided in Eqs. (29) and (30), yet physically it refers only to the $u \to \infty$ limit. Such an amplitude describes both electron and rotated-electron occupancies, which in that limit are similar quantum particles.

The expressions given in Eqs. (20)-(30) uniquely define the matrix elements between Bethe states of the electron - rotated-electron unitary operator considered here.

4. The unitary-operator matrix elements between energy eigenstates beyond the BA solution

Here we derive the expression of the electron - rotated-electron unitary operator matrix elements between energy eigenstates beyond the BA solution. For those the numbers n_η and n_s of Eq. (7) have finite values.

We start by showing that the six generators of the global η-spin and spin $SU(2)$ symmetries commute with the electron - rotated-electron unitary operator. To achieve that goal, it is useful to express the kinetic-energy operator

$\hat{T}$ given in Eq. (2) as $\hat{T} = \hat{T}_0 + \hat{T}_{+1} + \hat{T}_{-1}$. Here,

$$\hat{T}_\gamma = -\sum_{\langle j,j' \rangle} \hat{T}_{\gamma;,j,j'}\,, \quad \gamma = 0, \pm 1\,,$$

$$\hat{T}_{0;j,j'} = \sum_\sigma [\hat{n}_{j,-\sigma}\, c_{j,\sigma}^\dagger\, c_{j',\sigma}\, \hat{n}_{j',-\sigma} + (1 - \hat{n}_{j,-\sigma})\, c_{j,\sigma}^\dagger\, c_{j',\sigma}\, (1 - \hat{n}_{j',-\sigma}) + c.c.]\,,$$

$$\hat{T}_{+1;j,j'} = \sum_\sigma [\hat{n}_{j,-\sigma}\, c_{j,\sigma}^\dagger\, c_{j',\sigma}\, (1 - \hat{n}_{j',-\sigma}) + \hat{n}_{j',-\sigma}\, c_{j',\sigma}^\dagger\, c_{j,\sigma}\, (1 - \hat{n}_{j,-\sigma})]\,,$$

$$\hat{T}_{-1;j,j'} = \sum_\sigma [(1 - \hat{n}_{j,-\sigma})\, c_{j,\sigma}^\dagger\, c_{j',\sigma}\, \hat{n}_{j',-\sigma} + (1 - \hat{n}_{j',-\sigma})\, c_{j',\sigma}^\dagger\, c_{j,\sigma}\, \hat{n}_{j,-\sigma}]\,. \tag{33}$$

While the operator $\hat{T}_0$ does not change electron double occupancy, the operators $\hat{T}_{+1}$ and $\hat{T}_{-1}$ change it by $+1$ and -1, respectively.

For $u > 0$ the expression of the operator $\hat{S}$ such that $\hat{V} = e^{-\hat{S}}$ can be expanded in a series of t/U,

$$\hat{S} = -\frac{t}{U} \left[\hat{T}_{+1} - \hat{T}_{-1} \right] + \mathcal{O}(t^2/U^2)\,. \tag{34}$$

Although there are infinite choices for the operators $\hat{V} = e^{-\hat{S}}$ and $\hat{S}$, they share two important properties [19, 37, 38]: (i) To leading order in t/U all read $-\frac{t}{U} [\hat{T}_{+1} - \hat{T}_{-1}]$, as given in Eq. (34); (ii) Their operational expressions involve only the kinetic operators $\hat{T}_0$, $\hat{T}_{+1}$, and $\hat{T}_{-1}$ of Eq. (33). Such exact properties apply to the specific electron - rotated-electron unitary operator $\hat{V}$ considered here. Since it commutes with itself, the equalities $\hat{V} = e^{-\hat{S}} = \tilde{V} = e^{-\tilde{S}}$ and $\hat{S} = \tilde{S}$ hold. Hence both the operators $\hat{V}$ and $\hat{S}$ have the same expression in terms of electron and rotated-electron creation and annihilation operators, so that,

$$\tilde{S} = -\frac{t}{U} \left[\tilde{T}_{+1} - \tilde{T}_{-1} \right] + \dots\,. \tag{35}$$

However, although $\hat{S} = \tilde{S}$, except for $u \to \infty$ one has that $\hat{T}_0 \neq \tilde{T}_0$, $\hat{T}_{+1} \neq \tilde{T}_{+1}$, and $\hat{T}_{-1} \neq \tilde{T}_{-1}$ where,

$$\tilde{T}_\gamma = -\sum_{\langle j,j' \rangle} \tilde{T}_{\gamma;,j,j'}\,, \quad \gamma = 0, \pm 1\,,$$

$$\tilde{T}_{0;j,j'} = \sum_\sigma [\tilde{n}_{j,-\sigma}\, \tilde{c}_{j,\sigma}^\dagger\, \tilde{c}_{j',\sigma}\, \tilde{n}_{j',-\sigma} + (1 - \tilde{n}_{j,-\sigma})\, \tilde{c}_{j,\sigma}^\dagger\, \tilde{c}_{j',\sigma}\, (1 - \tilde{n}_{j',-\sigma}) + c.c.]\,,$$

$$\tilde{T}_{+1;j,j'} = \sum_\sigma [\tilde{n}_{j,-\sigma}\, \tilde{c}_{j,\sigma}^\dagger\, \tilde{c}_{j',\sigma}\, (1 - \tilde{n}_{j',-\sigma}) + \tilde{n}_{j',-\sigma}\, \tilde{c}_{j',\sigma}^\dagger\, \tilde{c}_{j,\sigma}\, (1 - \tilde{n}_{j,-\sigma})]\,,$$

$$\tilde{T}_{-1;j,j'} = \sum_\sigma [(1 - \tilde{n}_{j,-\sigma})\, \tilde{c}_{j,\sigma}^\dagger\, \tilde{c}_{j',\sigma}\, \tilde{n}_{j',-\sigma} + (1 - \tilde{n}_{j',-\sigma})\, \tilde{c}_{j',\sigma}^\dagger\, \tilde{c}_{j,\sigma}\, \tilde{n}_{j,-\sigma}]\,. \tag{36}$$

Furthermore, for finite u values one has that $-\frac{t}{U} [\hat{T}_{+1} - \hat{T}_{-1}] \neq -\frac{t}{U} [\tilde{T}_{+1} - \tilde{T}_{-1}]$. The equality $\hat{S} = \tilde{S}$ refers to the full expansion in terms of the two sets of three operators $\hat{T}_0$, $\hat{T}_{+1}$, $\hat{T}_{-1}$ and $\tilde{T}_0$, $\tilde{T}_{+1}$, $\tilde{T}_{-1}$, respectively. Only performing the sum of the infinite terms of the corresponding two expansions does that equality holds.

To confirm that the three generators of the spin $SU(2)$ symmetry, three generators of the η-spin $SU(2)$ symmetry, and the momentum operator $\hat{P}$ commute with the electron - rotated-electron unitary operator $\hat{V} = \tilde{V}$, one uses the exact result that the unitary operator $\hat{V}$ can be solely expressed in terms of the three kinetic operators given in Eq. (33) [19, 37]. In Ref. [19] the following twenty one commutators were found to vanish,

$$[\hat{P}, \hat{T}_l] = [\hat{S}_\alpha^{x_3}, \hat{T}_l] = [\hat{S}_\alpha^\pm, \hat{T}_l] = 0\,; \quad \alpha = \eta, s\,, \ l = 0, \pm 1\,. \tag{37}$$

Although the algebra involved in their derivation is cumbersome, it is straightforward. The vanishing of such commutators then implies that the momentum operator and the six generators of the η-spin and spin algebras commute with the unitary operator $\hat{V}$,

$$[\hat{P}, \hat{V}] = [\hat{S}_\alpha^{x_3}, \hat{V}] = [\hat{S}_\alpha^\pm, \hat{V}] = 0\,; \quad \alpha = \eta, s\,. \tag{38}$$

Expression of a general operator $\hat{O}$ in terms of rotated-electron creation and annihilation operators includes a set of commutators involving the operators $\tilde{O} = \hat{V}^\dagger \hat{O} \hat{V}$ and $\tilde{S}$. It reads,

$$\hat{O} = \tilde{O} + [\tilde{O}, \tilde{S}] + \frac{1}{2} [[\tilde{O}, \tilde{S}], \tilde{S}] + \dots\,. \tag{39}$$

Combination of this general operator expression with the vanishing commutators of Eq. (38) confirms that the momentum operator and the six generators of the spin and η-spin $SU(2)$ symmetries have the same expression in terms of electron and rotated-electron creation and annihilation operators. Specifically, the momentum operator reads,

$$\hat{P} = \sum_{\sigma=\uparrow,\downarrow} \sum_k k\, c^\dagger_{k,\sigma}\, c_{k,\sigma} = \tilde{P} = \sum_{\sigma=\uparrow,\downarrow} \sum_k k\, \tilde{c}^\dagger_{k,\sigma}\, \tilde{c}_{k,\sigma}\,. \tag{40}$$

Furthermore, the six generators of the partial $SO(4)$ symmetry contained in the model global symmetry are given by,

$$\hat{S}^{x_3}_\alpha = \sum_{j=1}^{N_a} \hat{s}^{x_3}_{j,\alpha} = \tilde{S}^{x_3}_\alpha = \sum_{j=1}^{N_a} \tilde{s}^{x_3}_{j,\alpha}\,, \quad \alpha=\eta,s\,,$$

$$\hat{S}^\pm_\alpha = \sum_{j=1}^{N_a} \hat{s}^\pm_{j,\alpha} = \tilde{S}^\pm_\alpha = \sum_{j=1}^{N_a} \tilde{s}^\pm_{j,\alpha}\,, \quad \alpha=\eta,s\,. \tag{41}$$

Here the local operators read,

$$\hat{s}^{x_3}_{j,\eta} = -\frac{1}{2}(1-\hat{n}_{j,\uparrow}-\hat{n}_{j,\downarrow})\,; \quad \hat{s}^+_{j,\eta} = (-1)^j\, c^\dagger_{j,\downarrow}\, c^\dagger_{j,\uparrow}\,; \quad \hat{s}^-_{j,\eta} = (-1)^j\, c_{j,\uparrow}\, c_{j,\downarrow}\,,$$

$$\hat{s}^{x_3}_{j,s} = -\frac{1}{2}(\hat{n}_{j,\uparrow}-\hat{n}_{j,\downarrow})\,; \quad \hat{s}^+_{j,s} = c^\dagger_{j,\downarrow}\, c_{j,\uparrow}\,; \quad \hat{s}^-_{j,s} = c^\dagger_{j,\uparrow}\, c_{j,\downarrow}\,. \tag{42}$$

The corresponding rotated local operators $\tilde{s}^l_{j,\eta}$ and $\tilde{s}^l_{j,s}$ where $l=x_3,\pm$ are given below. They have similar expressions, except that the electron creation and annihilation operators are replaced by rotated-electron creation and annihilation operators, respectively.

The seventh generator of the model global $[SU(2)\otimes SU(2)\otimes U(1)]/Z_2^2 = SO(3)\otimes SO(3)\otimes U(1)$ symmetry, which is that of the global c hidden $U(1)$ symmetry, Eq. (3), can be written in terms of the rotated-electron number operators $\tilde{n}_{j,\sigma} = \tilde{c}^\dagger_{j,\sigma}\tilde{c}_{j,\sigma}$ given in Eq. (16) as follows,

$$2\tilde{S}_c = \sum_{j=1}^{N_a} \tilde{s}_{j,c}\,; \quad \tilde{s}_{j,c} = \sum_{\sigma=\uparrow,\downarrow} \tilde{n}_{j,\sigma}\,(1-\tilde{n}_{j,-\sigma})\,. \tag{43}$$

For $u>0$ it commutes with the 1D Hubbard model [19]. On the other hand, except in the $u\to\infty$ limit and in contrast to the remaining six generators provided in Eq. (41), the generator of the c hidden $U(1)$ symmetry given here does not commute with the unitary operator $\hat{V}$. This is behind the hidden character of such a symmetry.

The six local operators $\hat{s}^l_{j,\alpha}$, where $\alpha=\eta,s$ and $l=x_3,\pm$, and the also unrotated local operator $\hat{s}_{j,c} = \sum_{\sigma=\uparrow,\downarrow} \hat{n}_{j,\sigma}\,(1-\hat{n}_{j,-\sigma})$ commute with the Hamiltonian electron-interaction operator $\hat{V}_D$ provided in Eq. (2),

$$[\hat{V}_D, \hat{s}^l_{j,\alpha}] = [\hat{V}_D, \hat{s}_{j,c}] = 0\,, \quad \alpha=\eta,s\,. \tag{44}$$

Indeed, such seven local operators are the generators of the local gauge $SU(2)\otimes SU(2)\otimes U(1)$ symmetry of the Hubbard Hamiltonian at $t=0$ [36].

That the electron - rotated-electron unitary operator $\hat{V}$ commutes with the six generators of the global η-spin and spin $SU(2)$ symmetries implies that its following matrix elements between energy eigenstates have the same value,

$$\langle \Psi_{l_o,l_\triangle,u} | \hat{V} | \Psi_{l',l_\triangle,u} \rangle = \langle \Psi_{l_o,l^0_\triangle,u} | \hat{V} | \Psi_{l',l^0_\triangle,u} \rangle\,,$$

$$|\Psi_{l_o,l_\triangle,u}\rangle = \prod_{\alpha=\eta,s} \left[\frac{1}{\sqrt{\mathcal{C}_\alpha}} (\hat{S}^+_\alpha)^{n_\alpha} \right] |\Psi_{l_o,l^0_\triangle,u}\rangle\,,$$

$$|\Psi_{l',l_\triangle,u}\rangle = \prod_{\alpha=\eta,s} \left[\frac{1}{\sqrt{\mathcal{C}_\alpha}} (\hat{S}^+_\alpha)^{n_\alpha} \right] |\Psi_{l',l^0_\triangle,u}\rangle\,. \tag{45}$$

This holds for the set of energy eigenstates $\{|\Psi_{l_o,l_\triangle,u}\rangle\}$ and $\{|\Psi_{l',l_\triangle,u}\rangle\}$ with the same $l_\triangle$ values and thus $n_\eta=1,...,2S_\eta$ and $n_s=1,...,2S_s$ values. This matrix-element equality is confirmed on replacing $(\hat{S}^-_\alpha)^{n_\alpha}\hat{V}(\hat{S}^+_\alpha)^{n_\alpha}$ by $(\hat{S}^-_\alpha\,\hat{S}^+_\alpha)^{n_\alpha}\hat{V}$

in the matrix elements of Eq. (45) and systematically using the $SU(2)$ algebra commutator $[\hat{S}_\alpha^-, \hat{S}_{\alpha'}^+] = -2\delta_{\alpha,\alpha'}\hat{S}_\alpha^{x_3}$ until reaching the following expressions,

$$
\begin{aligned}
\langle\Psi_{l_o,l_\triangle,u}|\hat{V}|\Psi_{l',l_\triangle,u}\rangle &= \prod_{\alpha=\eta,s}\frac{1}{\mathcal{C}_\alpha}\langle\Psi_{l_o,l_\triangle^0,u}|(\hat{S}_\alpha^-\,\hat{S}_\alpha^+)^{n_\alpha}\hat{V}|\Psi_{l',l_\triangle^0,u}\rangle \\
&= \prod_{\alpha=\eta,s}\frac{1}{\mathcal{C}_\alpha}\langle\Psi_{l_o,l_\triangle^0,u}|(\delta_{n_\alpha,0}+[n_\alpha!]\prod_{j'=1}^{n_\alpha}[2S_\alpha+1-j'])\hat{V}|\Psi_{l',l_\triangle^0,u}\rangle \\
&= \langle\Psi_{l_o,l_\triangle^0,u}|\hat{V}|\Psi_{l',l_\triangle^0,u}\rangle\,.
\end{aligned}
\tag{46}
$$

Equation (14) was used to arrive to the last expression. Note that this is the same algebra as that behind the normalization of an energy eigenstate $|\Psi_{l_o,l_\triangle,u}\rangle$,

$$
\begin{aligned}
\langle\Psi_{l_o,l_\triangle,u}|\Psi_{l_o,l_\triangle,u}\rangle &= \prod_{\alpha=\eta,s}\frac{1}{\mathcal{C}_\alpha}\langle\Psi_{l_o,l_\triangle^0,u}|(\hat{S}_\alpha^-\,\hat{S}_\alpha^+)^{n_\alpha}|\Psi_{l_o,l_\triangle^0,u}\rangle \\
&= \prod_{\alpha=\eta,s}\frac{1}{\mathcal{C}_\alpha}\langle\Psi_{l_o,l_\triangle^0,u}|(\delta_{n_\alpha,0}+[n_\alpha!]\prod_{j'=1}^{n_\alpha}[2S_\alpha+1-j'])|\Psi_{l_o,l_\triangle^0,u}\rangle \\
&= \langle\Psi_{l_o,l_\triangle^0,u}|\Psi_{l_o,l_\triangle^0,u}\rangle = 1\,.
\end{aligned}
\tag{47}
$$

The matrix-element equalities given in Eq. (46) are consistent with the properties of the general amplitudes $\langle x_1,...,x_N;y_1,...,y_{N_\downarrow}|\Psi_{l_o,l_\triangle,u}\rangle$. The latter are closely related to the amplitude $\langle x_1,...,x_{N^0};y_1,...,y_{N_\downarrow^0}|\Psi_{l_o,l_\triangle^0,u}\rangle$ of the initial Bethe state $|\Psi_{l_o,l_\triangle^0,u}\rangle$ of Eq. (45). This follows from the invariance under the electron - rotated-electron unitary transformation of the η-spin and spin degrees of freedom of the rotated-electron occupancy configurations that generate the non-LWSs $|\Psi_{l_o,l_\triangle,u}\rangle$. Out of the $N = N^0 + 2n_\eta$ electrons of the latter states, except for an overall phase factor $(-1)^{n_\eta}$, the amplitudes $\langle x_1,...,x_N;y_1,...,y_{N_\downarrow}|\Psi_{l_o,l_\triangle,u}\rangle$ are insensitive to the spatial coordinates of the n_η on-site electron pairs originated from n_η unoccupied sites of the initial Bethe state $|\Psi_{l_o,l_\triangle^0,u}\rangle$. Furthermore, out of the $N_\downarrow = N_\downarrow^0 + n_\eta + n_s$ down-spin electrons of the non-LWSs $|\Psi_{l_o,l_\triangle,u}\rangle$, such amplitudes are insensitive to both the spatial coordinates of the n_η spin-down electrons in the on-site electron pairs originated from n_η unoccupied sites of the initial Bethe state $|\Psi_{l_o,l_\triangle^0,u}\rangle$ and the n_s spin-down electrons generated by n_s spin-flip processes of n_s spin-up electrons of the same initial Bethe state. Hence the amplitudes $\langle x_1,...,x_N;y_1,...,y_{N_\downarrow}|\Psi_{l_o,l_\triangle,u}\rangle$ only depend on the spatial coordinates $x_1,...,x_{N_a-2S_\eta}$ of the initial $N^0 = [N_a - 2S_\eta]$ electrons that are not generated from η-spin-flip processes and on those $y_1,...,y_{N_a/2-S_\eta-S_s}$ of the initial $N_\downarrow^0 = \frac{N_a}{2} - S_\eta - S_s$ spin-down electrons that are not generated from spin-flip processes. Hence they may be rather rewritten as $\langle x_1,...,x_{N_a-2S_\eta};y_1,...,y_{N_a/2-S_\eta-S_s}|\Psi_{l_o,l_\triangle,u}\rangle$ and read,

$$
\begin{aligned}
&f_{l_o,l_\triangle,u}(x_1,...,x_{N_a-2S_\eta};y_1,...,y_{N_a/2-S_\eta-S_s}) = \\
&\langle x_1,...,x_{N_a-2S_\eta};y_1,...,y_{N_a/2-S_\eta-S_s}|\Psi_{l_o,l_\triangle,u}\rangle = \\
&(-1)^{n_\eta}\,f_{l_o,l_\triangle^0,u}(x_1,...,x_{N^0};y_1,...,y_{N_\downarrow^0})|_{N^0=N_a-2S_\eta\,;N_\downarrow^0=N_a/2-S_\eta-S_s}\,.
\end{aligned}
\tag{48}
$$

Here the Bethe-state electron amplitudes $f_{l_o,l_\triangle^0,u}(x_1,...,x_{N^0};y_1,...,y_{N_\downarrow^0})$ are those of Eqs. (25)-(28).

A similar analysis of the rotated-electron amplitudes involving the non-LWSs $|\Psi_{l_o,l_\triangle,u}\rangle$ leads to,

$$
\begin{aligned}
&f_{l_o,l_\triangle,rt}(x_1^s,...,x_{N_R^s}^s;x_1^d,...,x_{N_{R,-1/2}^{\eta,0}}^d;x_1^{s\downarrow},...,x_{N_{R,-1/2}^{s,0}}^{s\downarrow}) = \\
&\langle u;x_1^s,...,x_{N_R^s}^s;x_1^d,...,x_{N_{R,-1/2}^{\eta,0}}^d;x_1^{s\downarrow},...,x_{N_{R,-1/2}^{s,0}}^{s\downarrow}|\Psi_{l_o,l_\triangle,u}\rangle = \\
&(-1)^{n_\eta}\,f_{l_o,l_\triangle^0,rt}(x_1^s,...,x_{N_R^s}^s;x_1^d,...,x_{N_{R,-1/2}^{\eta,0}}^d;x_1^{s\downarrow},...,x_{N_{R,-1/2}^{s,0}}^{s\downarrow})\,,
\end{aligned}
\tag{49}
$$

where the Bethe-state rotated-electron amplitudes $f_{l_o,l_\triangle^0,rt}(x_1^s,...,x_{N_R^s}^s;x_1^d,...,x_{N_{R,-1/2}^{\eta,0}}^d;x_1^{s\downarrow},...,x_{N_{R,-1/2}^{s,0}}^{s\downarrow})$ are those of Eqs. (29)-(31).

The energy eigenstates $|\Psi_{l_o,l_\triangle,u}\rangle$ may now be written in two alternative representations as,

$$
\begin{aligned}
|\Psi_{l_o,l_\triangle,u}\rangle &= \sum_{1\leq x_i\leq N_a} f_{l_o,l_\triangle,u}(x_1,...,x_{N_a-2S_\eta};y_1,...,y_{N_a/2-S_\eta-S_s})|x_1,...,x_{N_a-2S_\eta};y_1,...,y_{N_a/2-S_\eta-S_s}\rangle, \\
&= \sum_{1\leq x_i\leq N_a} f_{l_o,l_\triangle,rt}(x_1^s,...,x_{N_R^s}^s;x_1^d,...,x_{N_{R,-1/2}^{\eta,0}}^d;x_1^{s\downarrow},...,x_{N_{R,-1/2}^{s,0}}^{s\downarrow}) \\
&\times \ |u;x_1^s,...,x_{N_R^s}^s;x_1^d,...,x_{N_{R,-1/2}^{\eta,0}}^d;x_1^{s\downarrow},...,x_{N_{R,-1/2}^{s,0}}^{s\downarrow}\rangle,
\end{aligned}
\tag{50}
$$

respectively. In both cases the summation is over all $x_1,...,x_{N_a-2S_\eta}$ from 1 to N_a.

The alternative expressions provided in Eq. (50) apply to all 4^{N_a} energy eigenstates, including the Bethe states. From the above results one finds that the electron - rotated-electron unitary operator matrix element between two arbitrary energy eigenstates out of the 4^{N_a} such states that span the Hilbert space is given by,

$$
\begin{aligned}
\langle\Psi_{l_o,l_\triangle,u}|\hat{V}|\Psi_{l',l'_{\eta s},u}\rangle &= \langle\Psi_{l_o,l_\triangle,u}|\Psi_{l',l'_\triangle,\infty}\rangle = \delta_{l_\triangle,l'_\triangle}\, V_{l_o,l'_o} \\
&= \delta_{l_\triangle,l'_\triangle} \sum_{1\leq x_i\leq N_a} f_{l_o,l_\triangle,u}^*(x_1,...,x_{N_a-2S_\eta};y_1,...,y_{N_a/2-S_\eta-S_s}) \\
&\times \ f_{l',l_\triangle,\infty}(x_1,...,x_{N_a-2S_\eta};y_1,...,y_{N_a/2-S_\eta-S_s}).
\end{aligned}
\tag{51}
$$

Here the amplitudes are those given in Eq. (49). Note that both amplitudes refer to the same n_η value. Hence the product of the two phase factors of the form $(-1)^{n_\eta}$ appearing in Eq. (49) gives 1. This together with the amplitude expression provided in that equation is fully consistent with the matrix-element equalities of Eq. (45).

The matrix element provided in Eq. (51) can alternatively be expressed in terms of the rotated-electron amplitudes, as in Eq. (24) for the Bethe states, with the result,

$$
\begin{aligned}
\langle\Psi_{l_o,l_\triangle,u}|\hat{V}|\Psi_{l',l'_{\eta s},u}\rangle &= \langle\Psi_{l_o,l_\triangle,u}|\Psi_{l',l'_\triangle,\infty}\rangle = \delta_{l_\triangle,l'_\triangle}\, V_{l_o,l'_o} \\
&= \delta_{l_\triangle,l'_\triangle} \sum_{1\leq x_i\leq N_a}\sum_{1\leq x'_i\leq N_a} f_{l_o,l_\triangle,rt}^*(x_1^s,...,x_{N_R^s}^s;x_1^d,...,x_{N_{R,-1/2}^{\eta,0}}^d;x_1^{s\downarrow},...,x_{N_{R,-1/2}^{s,0}}^{s\downarrow}) \\
&\times \ f_{l',l_\triangle,rt}(x_1^{s\prime},...,x_{N_R^s}^{s\,\prime};x_1^{d\prime},...,x_{N_{R,-1/2}^{\eta,0}}^{d}{}';x_1^{s\downarrow\prime},...,x_{N_{R,-1/2}^{s,0}}^{s\downarrow}{}') \\
&\times \ \langle u;x_1^s,...,x_{N_R^s}^s;x_1^d,...,x_{N_{R,-1/2}^{\eta,0}}^d;x_1^{s\downarrow},...,x_{N_{R,-1/2}^{s,0}}^{s\downarrow}| \\
&\times \ |\infty;x_1^{s\prime},...,x_{N_R^s}^{s\,\prime};x_1^{d\prime},...,x_{N_{R,-1/2}^{\eta,0}}^{d}{}';x_1^{s\downarrow\prime},...,x_{N_{R,-1/2}^{s,0}}^{s\downarrow}{}'\rangle.
\end{aligned}
\tag{52}
$$

For all 4^{N_a} energy eigenstates $|\Psi_{l,l'_{\eta s},u}\rangle$ the rotated-electron amplitudes appearing here are given by,

$$
\begin{aligned}
&f_{l_o,l_\triangle,rt}(x_1^s,...,x_{N_R^s}^s;x_1^d,...,x_{N_{R,-1/2}^{\eta,0}}^d;x_1^{s\downarrow},...,x_{N_{R,-1/2}^{s,0}}^{s\downarrow}) = \\
&\mathcal{C}_{rt}\,[\phi_{U(1)}^c(x_1^s,...,x_{N_R^s}^s)\times\phi_{SU(2)}^\eta(x_1^d,x_2^d,...,x_{N_{R,-1/2}^{\eta,0}}^d)\times\phi_{SU(2)}^s(x_1^{s\downarrow},...,x_{N_{R,-1/2}^{s,0}}^{s\downarrow})],
\end{aligned}
\tag{53}
$$

where,

$$
\begin{aligned}
\phi_{U(1)}^c(x_1^s,...,x_{N_R^s}^s) &= (-1)^Q\left[\sum_P(-1)^P e^{i\sum_{j=1}^{2S_c}k_{Pj}x_{Qj}^s}\right] = (-1)^Q\,\det\left[e^{ik_{Pj}x_{Qj}^s}\right], \\
\phi_{SU(2)}^\eta(x_1^d,x_2^d,...,x_{N_{R,-1/2}^{\eta,0}}^d) &= (-1)^{[N_a-2S_c-2S_\eta+2n_\eta]/2}\,\phi_1(x_1^d,x_2^d,...,x_{N_{R,-1/2}^{\eta,0}}^d), \\
\phi_{SU(2)}^s(x_1^{s\downarrow},...,x_{N_{R,-1/2}^{s,0}}^{s\downarrow}) &= \phi_2(x_1^{s\downarrow},...,x_{N_{R,-1/2}^{s,0}}^{s\downarrow}).
\end{aligned}
\tag{54}
$$

Except for the extra phase factor $(-1)^{n_\eta}$ in the function $\phi_{SU(2)}^\eta(x_1^d,x_2^d,...,x_{N_{R,-1/2}^{\eta,0}}^d)$, the quantities appearing in Eqs. (53) and (54) are the same as in Eqs. (29) and (30) for the Bethe states. Those given here are valid for both the latter states and the non-LWSs generated from them.

The alternative general expressions provided in Eqs. (51) and (52) for the $4^{N_a}\times 4^{N_a}$ matrix elements between arbitrary energy eigenstates along with Eqs. (25)-(28), (48)-(49), and (53)-(54) for the corresponding amplitudes uniquely define the electron - rotated-electron unitary operator and corresponding unitary transformation considered

in this paper. In the $u \to \infty$ limit rotated electrons become electrons, so that the electron - rotated-electron unitary operator becomes the unity operator. Consistent, analysis of the amplitude behavior confirms that in such a limit the matrix elements given in Eqs. (51) and (52) simplify to,

$$\lim_{u \to \infty} \langle \Psi_{l_o, l_\triangle, u} | \hat{V} | \Psi_{l', l'_{\eta s}, u} \rangle = \delta_{l_\triangle, l'_\triangle} \lim_{u \to \infty} V_{l_o, l'_o} = \delta_{l_\triangle, l'_\triangle} \delta_{l_o, l'_o} \,. \tag{55}$$

III.   THE THREE ELEMENTARY OBJECTS WHOSE OCCUPANCY CONFIGURATIONS GENERATE THE EXACT ENERGY EIGENSTATES

Here we show that all 4^{N_a} energy eigenstates are generated by occupancy configurations of three rotated-electron related elementary objects: the η-spin-less and spin-less c fermions, η-spin-1/2 η-spinons, and spin-1/2 spinons.

A.   Elementary quantum object operators emerging from the model algebraic structure and symmetries

The local generator $\hat{s}_{j,c} = \sum_{\sigma=\uparrow,\downarrow} \hat{n}_{j,\sigma} (1 - \hat{n}_{j,-\sigma})$ given in Eq. (43) and the alternative local generator $\hat{s}^h_{j,c} = (1 - \hat{s}_{j,c})$ of the Hamiltonian electron-interaction term gauge $U(1)$ symmetry in $SU(2) \otimes SU(2) \otimes U(1)$ may be expressed as,

$$\hat{s}_{j,c} = \hat{n}_{j,c} = \hat{f}^\dagger_{j,c} \hat{f}_{j,c} \,; \qquad \hat{s}^h_{j,c} = (1 - \hat{n}_{j,c}) = \hat{f}_{j,c} \hat{f}^\dagger_{j,c} \,. \tag{56}$$

Here $\hat{f}^\dagger_{j,c}$ and $\hat{f}_{j,c}$ stand for the following creation and annihilation operators, respectively, of suitable spin-less and η-spin-less fermions,

$$\begin{aligned} \hat{f}^\dagger_{j,c} &= c^\dagger_{j,\sigma} (1 - \hat{n}_{j,-\sigma}) + (-1)^j c_{j,\sigma} \hat{n}_{j,-\sigma} \,, \\ \hat{f}_{j,c} &= c_{j,\sigma} (1 - \hat{n}_{j,-\sigma}) + (-1)^j c^\dagger_{j,\sigma} \hat{n}_{j,-\sigma} \,, \quad \mathcal{J} = (3/2 - \sigma) = 1, 2 \,. \end{aligned} \tag{57}$$

This equation refers to two representations for the spin-less and η-spin-less fermions, which we call $\mathcal{J} = (3/2 - \sigma) = 1, 2$ representations. As confirmed below, the monodromy matrix of the BA inverse-scattering method [4, 41–43] contains $\hat{f}^\dagger_{j,c}$ and $\hat{f}_{j,c}$ operators referring to the two $\mathcal{J} = 1, 2$ representations. The 1 representation (and the 2 representation) corresponds to the choice $\sigma = \uparrow$ (and $\sigma = \downarrow$) in Eq. (57). However, the fermions whose operators are given in Eq. (57) are spin-less and η-spin-less objects that do not carry spin σ. Both representations are faithful, being alternative.

The exact solution of 1D integrable models can be reached by two different methods: The coordinate BA used by Bethe himself [44] and the more algebraic operator formulation, usually called inverse scattering method [45]. For the 1D Hubbard model such an algebraic formulation of the Bethe states refers to the transfer matrix of the classical coupled spin model, which is its "covering" [41, 42]. It is not among the goals of this paper to provide full details about the algebraic inverse-scattering BA method. One of its properties is that before arriving to the same BA equations as the coordinate BA, the former method involves creation and annihilation fields that act onto an extended and partially unphysical Hilbert space, larger than that of the 1D Hubbard model [3, 4]. The two types of operators given in Eq. (57) associated with the $\mathcal{J} = 1, 2$ representations, respectively, act onto that extended Hilbert space. Within the inverse-scattering BA method, the unwanted and unphysical terms are eliminated by imposing suitable restrictions to the rapidities that change the nature of the fields. Such a procedure is equivalent to project the problem onto the model smaller physical Hilbert space.

Concerning the operators $\hat{f}^\dagger_{j,c}$ and $\hat{f}_{j,c}$, such restrictions impose the use of only one of the above $\mathcal{J} = 1, 2$ representations. Therefore and except for the on-site L-matrices general expression, in this paper we consider only the $\mathcal{J} = 1$ representation such that,

$$\begin{aligned} \hat{f}^\dagger_{j,c} &= c^\dagger_{j,\uparrow} (1 - \hat{n}_{j,\downarrow}) + (-1)^j c_{j,\uparrow} \hat{n}_{j,\downarrow} \,, \\ \hat{f}_{j,c} &= c_{j,\uparrow} (1 - \hat{n}_{j,\downarrow}) + (-1)^j c^\dagger_{j,\uparrow} \hat{n}_{j,\downarrow} \,. \end{aligned} \tag{58}$$

Within the inverse scattering method [3, 4, 43], the central object to be diagonalized is the quantum transfer matrix, rather than the underlying 1D Hubbard model. The transfer-matrix eigenvalues provide the spectrum of a set of generalized conserved charges [41–43]. From the point of view of the BA algebraic inverse-scattering method, a central role is ascribed to the monodromy matrix. (For further details on that matrix, see Refs. [4, 41–43].) The

monodromy matrix $\mathcal{T}_{j,j'}(\lambda)$ corresponding to site indices $j > j'$ where $j, j' = 1, ..., N_a$ can be expressed as a product of on-site L-matrices $\mathcal{L}_j(\lambda)$ as follows,

$$\mathcal{T}_{j,j'}(\lambda) = \prod_{j''=1}^{j-j'} \mathcal{L}_{j-j''}(\lambda), \quad j > j'. \tag{59}$$

The spectral parameter λ in the argument of $\mathcal{L}_j(\lambda)$ and $\mathcal{T}_{j,j'}(\lambda)$ parametrizes the Boltzmann weights [4]. For the 1D Hubbard model a pseudo-vacuum state exists, on which the monodromy matrix acts as a lower triangular matrix. Such a state is an eigenstate of its diagonal elements. This has enabled the algebraic construction of the Bethe states [3, 4], similar to those previously obtained by the coordinate BA [1, 2].

In the algebraic construction of the Bethe states program carried out in Refs. [3, 4], the charge and spin degrees of freedom were solved into two separated steps, respectively. That has decoupled the monodromy matrix problem into that of two matrices, referring to the charge and spin degrees of freedom, respectively. The studies of Refs. [3, 4] used the HWS formulation of the BA. To solve the charge problem a one-site doubly occupied state, which here we denote by $|j, \uparrow\downarrow\rangle$, was used as local reference state. (Within our LWS formulation, a similar procedure involves instead a one-site unoccupied state, which we call $|j, \odot\rangle$.) The corresponding global reference state $|\uparrow\downarrow\rangle$ was then defined by the tensor product $|\uparrow\downarrow\rangle = \prod_{j=1}^{N_a} \otimes |j, \uparrow\downarrow\rangle$. The latter state is an eigenstate of the transfer matrix. Indeed the triangular property is easily extended to a corresponding charge monodromy matrix. Its off-diagonal entries are some of the creation and annihilation fields. Their application onto $|\uparrow\downarrow\rangle$ generates the charge degrees of freedom of the energy-eigenstate configurations. On the other hand, to solve the spin problem the authors of Refs. [3, 4] have used another BA. It is equivalent to the solution of the six-vertex model in the presence of inhomogeneities. The solution of the spin degrees of freedom involves the diagonalization of the auxiliary transfer matrix associated with a spin monodromy matrix [3, 4]. Again, the off-diagonal entries of that matrix play the role of the creation and annihilation fields that generate the spin degrees of freedom of the energy-eigenstate configurations.

The local gauge symmetry of the Hamiltonian electron-interaction term and the related model global symmetry must be explicit in the algebraic operator formulation of its solution. This is in part why the solution of the 1D Hubbard model by the algebraic inverse scattering method [3, 4] was achieved only thirty years after that of the coordinate BA [1, 2]. Indeed, it was expected that on decoupling the monodromy matrix problem into those of a charge and spin monodromy matrix, respectively, both such matrices would have the same traditional Faddeev-Zamolodchikov ABCD form, found previously for the related 1D spin-1/2 isotropic Heinsenberg model [26, 45]. Such a prediction followed the expected spin $SU(2)$ symmetry and η-spin charge $SU(2)$ symmetry associated with a model global $SO(4) = [SU(2) \otimes SU(2)]/Z_2$ symmetry [34]. If that was the global symmetry of the 1D Hubbard model, the charge and spin monodromy matrices would indeed have the same ABCD form.

Consistent with the local gauge $SU(2) \otimes SU(2) \otimes U(1)$ symmetry of the Hamiltonian electron-interaction term found in Ref. [36] and the related model global $SO(3) \otimes SO(3) \otimes U(1) = [SO(4) \otimes U(1)]/Z_2$ symmetry found more recently in Ref. [19], all tentative schemes using charge and spin monodromy matrices of the same ABCD form failed to achieve the BA equations obtained in Refs. [1, 2] by means of the coordinate BA. The problem was solved in Ref. [4], by use of an appropriate representation of the charge and spin monodromy matrices, which allows for possible *hidden symmetries*. Indeed, the structure of the charge and spin monodromy matrices reported in the latter reference is able to distinguish creation and annihilation fields as well as possible hidden symmetries. That for $u > 0$ the 1D Hubbard model spin and charge degrees of freedom are associated with the $SU(2)$ and $U(2) = SU(2) \otimes U(1)$ symmetries, respectively, in $[SU(2) \otimes U(2)]/Z_2^2 = SO(3) \otimes SO(3) \otimes U(1)$, rather than merely with two $SU(2)$ symmetries, is behind the different ABCD and ABCDF forms found in Refs. [3, 4] for the inverse-scattering method BA solution spin and charge monodromy matrices, respectively: Due to the extra $U(1)$ symmetry in $U(2) = SU(2) \otimes U(1)$, the latter matrix is larger than the former and involves more fields.

However, the various operators contained in the monodromy matrix enter in the expression for the Bethe states found in Ref. [4] in a complicated way. This renders difficult an intuitive physical interpretation. A full algebraic construction of the Bethe states as that carried out in that reference is not between the goals of this paper. A less ambitious yet related task performed in the following is the expression of the L-matrix $\mathcal{L}_j$ in the formal monodromy matrix expression provided in Eq. (59) in terms of *only* the seven generators of the local gauge $SU(2) \otimes SU(2) \otimes U(1)$ symmetry of the Hamiltonian electron-interaction term given in Eqs. (42) and (56) and related spin-less and η-spin-less fermion operators of Eq. (57). This confirms the important role played by that local symmetry and the related model global $[SU(2) \otimes SU(2) \otimes U(1)]/Z_2^2$ symmetry in the exact BA solution.

By combining that result with the requirement that the Bethe states must correspond to representations of the model global symmetry, we find that the generators of such states onto the electronic vacuum may be expressed in terms of a set of operators obtained by electron-rotating such seven generators and related spin-less and η-spin-less fermion operators. This confirms that although masked by the very complicated algebraic structure of the inverse-

scattering method, the BA solution performs the electron - rotated-electron unitary transformation defined in Section II B.

In the following we choose the same parameterizing functions $a = a(\lambda) = \cos\lambda$ and $b = b(\lambda) = \sin\lambda$ as in Refs. [4, 43]. Starting from the known expression of the on-site 4×4 L-matrix in terms of electron creation and annihilation operators, Eq. (A1) of Appendix A, after some algebra relying on Eqs. (42), (56), and (57) we arrive to the following remarkable expression for $\mathcal{L}_j$,

$$
\begin{bmatrix}
e^h \left[-iab + \frac{e^{i2\lambda}}{2}\hat{s}_{j,c}^h + \hat{s}_{j,\eta}^{x_3} \right] & -b\,\hat{f}_{j,c}\,\hat{n}_2^h - i(-1)^j a\,\hat{f}_{j,c}^\dagger\,\hat{n}_2 & ib\,\hat{f}_{j,c}\,\hat{n}_1^h - (-1)^j a\,\hat{f}_{j,c}^\dagger\,\hat{n}_1 & ie^h(-1)^j \hat{s}_{j,\eta}^- \\
-ib\,\hat{f}_{j,c}^\dagger\,\hat{n}_2^h + (-1)^j a\,\hat{f}_{j,c}\,\hat{n}_2 & -ie^{-h} \left[iab - \frac{e^{i2\lambda}}{2}\hat{s}_{j,c} + \hat{s}_{j,s}^{x_3} \right] & -e^{-h}\hat{s}_{j,s}^+ & ia\,\hat{f}_{j,c}\,\hat{n}_1^h + (-1)^j b\,\hat{f}_{j,c}^\dagger\,\hat{n}_1 \\
b\,\hat{f}_{j,c}^\dagger\,\hat{n}_1^h + i(-1)^j a\,\hat{f}_{j,c}\,\hat{n}_1 & e^{-h}\hat{s}_{j,s}^- & ie^{-h} \left[-iab + \frac{e^{i2\lambda}}{2}\hat{s}_{j,c} + \hat{s}_{j,s}^{x_3} \right] & a\,\hat{f}_{j,c}\,\hat{n}_2^h - i(-1)^j b\,\hat{f}_{j,c}^\dagger\,\hat{n}_2 \\
ie^h(-1)^j \hat{s}_{j,\eta}^+ & a\,\hat{f}_{j,c}^\dagger\,\hat{n}_1^h - i(-1)^j b\,\hat{f}_{j,c}\,\hat{n}_1 & ia\,\hat{f}_{j,c}^\dagger\,\hat{n}_2^h + (-1)^j b\,\hat{f}_{j,c}\,\hat{n}_2 & e^h \left[iab - \frac{e^{i2\lambda}}{2}\hat{s}_{j,c}^h + \hat{s}_{j,\eta}^{x_3} \right]
\end{bmatrix}
$$

$$
\sinh[2h] = \sinh[2h(\lambda)] = u\,2ab\,; \quad a = a(\lambda) = \cos\lambda\,; \quad b = b(\lambda) = \sin\lambda\,. \tag{60}
$$

Here $\hat{s}_{j,\eta}^l$ and $\hat{s}_{j,s}^l$ with $l = x_3, \pm$ are the local generators given in Eq. (42) of the two gauge $SU(2)$ symmetries, respectively. Moreover, $\hat{s}_{j,c}$ and $\hat{s}_{j,c}^h$ are the two alternative local generators defined in Eq. (56) of the gauge $U(1)$ symmetry in the $t = 0$ Hamiltonian gauge $SU(2) \otimes SU(2) \otimes U(1)$ symmetry. The operators $\hat{n}_2 = \hat{n}_{j,\uparrow}$, $\hat{n}_1^h = (1 - \hat{n}_1)$, and $\hat{n}_2^h = (1 - \hat{n}_2)$ multiplying the spin-less and η-spin-less fermion creation and annihilation operators select one of their expression two operator terms given in Eq. (57). To shorten the L-matrix $\mathcal{L}_j$ notation of Eq. (60), it is implicitly assumed that a spinless and η-spinless fermion operator multiplying an operator $\hat{n}_{\mathcal{J}}$ or $\hat{n}_{\mathcal{J}}^h$ with index $\mathcal{J} = 1$ (and $\mathcal{J} = 2$) corresponds to the 1 (and 2) representation of Eq. (57). The L-matrix $\mathcal{L}_j$ expression of Eq. (60) provides an explicit confirmation of the deep relation of the BA solution to the local gauge $SU(2) \otimes SU(2) \otimes U(1)$ symmetry of the Hamiltonian electron-interaction term associated with the vanishing commutators of Eq. (44).

We call c fermions the objects whose creation and annihilation operators $f_{j,c}^\dagger = \hat{V}^\dagger \hat{f}_{j,c}^\dagger \hat{V}$ and $f_{j,c} = \hat{V}^\dagger \hat{f}_{j,c} \hat{V}$, respectively, are generated from those of the spin-less and η-spin-less fermions of Eq. (58) by the electron - rotated-electron unitary transformation performed by the BA. Hence in terms of the corresponding rotated-electron creation and annihilation operators they read,

$$
\begin{aligned}
f_{j,c}^\dagger &= \tilde{c}_{j,\uparrow}^\dagger \,(1 - \tilde{n}_{j,\downarrow}) + (-1)^j\,\tilde{c}_{j,\uparrow}\,\tilde{n}_{j,\downarrow}\,, \\
f_{j,c} &= \tilde{c}_{j,\uparrow}\,(1 - \tilde{n}_{j,\downarrow}) + (-1)^j\,\tilde{c}_{j,\uparrow}^\dagger\,\tilde{n}_{j,\downarrow}\,.
\end{aligned} \tag{61}
$$

The c fermion local density operator is then given by,

$$
n_{j,c} = f_{j,c}^\dagger\, f_{j,c}\,. \tag{62}
$$

(Exceptionally, within our notation no upper index as in $f_{j,c}^\dagger$, $\tilde{f}$, and $\tilde{n}$ is used onto the (electron-rotated) c fermion operators $f_{j,c}$ and $n_{j,c}$, respectively.)

One may introduce corresponding c fermion momentum-dependent operators labeled by discrete momentum values q_j,

$$
f_{q_j,c}^\dagger = (f_{q_j,c})^\dagger = \frac{1}{\sqrt{N_a}} \sum_{j'=1}^{N_a} e^{+iq_j j'}\, f_{j',c}^\dagger\,; \quad j = 1, ..., N_a\,. \tag{63}
$$

For $N_a \gg 1$ and in units of $2\pi/N_a$, the discrete momentum values q_j are found below to be the quantum numbers of one of the BA excitation branches.

We consider as well the six rotated local operators $\tilde{s}_{j,\alpha}^l = \hat{V}^\dagger \hat{s}_{j,\alpha}^l \hat{V}$ with $\alpha = s, \eta$ and $l = x_3, \pm$. Those are generated from the remaining six generators of the local gauge $SU(2) \otimes SU(2) \otimes U(1)$ symmetry of the Hamiltonian electron-interaction term given in Eqs. (42),

$$
\begin{aligned}
\tilde{s}_{j,\eta}^{x_3} &= -\frac{1}{2}(1 - \tilde{n}_{j,\uparrow} - \tilde{n}_{j,\downarrow})\,; \quad \tilde{s}_{j,\eta}^+ = (-1)^j\,\tilde{c}_{j,\downarrow}^\dagger\,\tilde{c}_{j,\uparrow}^\dagger\,; \quad \tilde{s}_{j,\eta}^- = (-1)^j\,\tilde{c}_{j,\uparrow}\,\tilde{c}_{j,\downarrow}\,, \\
\tilde{s}_{j,s}^{x_3} &= -\frac{1}{2}(\tilde{n}_{j,\uparrow} - \tilde{n}_{j,\downarrow})\,; \quad \tilde{s}_{j,s}^+ = \tilde{c}_{j,\downarrow}^\dagger\,\tilde{c}_{j,\uparrow}\,; \quad \tilde{s}_{j,s}^- = \tilde{c}_{j,\uparrow}^\dagger\,\tilde{c}_{j,\downarrow}\,.
\end{aligned} \tag{64}
$$

The three rotated local spin operators $\tilde{s}^l_{j,s}$ and the three rotated local η-spin operators $\tilde{s}^l_{j,\eta}$ such that $l = \pm, x_3$ given here are associated with the spin-1/2 spinons and η-spin-1/2 η-spinons, respectively, as defined in this paper.

On the use of the general results of Ref. [19], one straightforwardly confirms that within the present operator formulation the site summation $\sum_{j=1}^{N_a}$ of the rotated local operators given in Eqs. (62) and (64) gives the seven generators of the model global $SO(3) \otimes SO(3) \otimes U(1) = [SU(2) \otimes SU(2) \otimes U(1)]/Z_2^2$ symmetry. For the six operators obtained under that site summation from the six rotated local operators of Eq. (64) that is readily confirmed by the form of the six generators of the model global symmetry provided in Eq. (41). On the other hand, concerning the generator of the global c hidden $U(1)$ symmetry given in Eq. (43), a straightforward operator algebra confirms that the c fermion local density operator (62) is the local operator $\tilde{s}_{j,c}$ appearing in Eq. (43). Hence the global c hidden $U(1)$ symmetry generator may be rewritten as,

$$2\tilde{S}_c = \sum_{j=1}^{N_a} n_{j,c} = \sum_{j=1}^{N_a} f^\dagger_{j,c} f_{j,c}. \tag{65}$$

The three local spinon operators $\tilde{s}^l_{j,s}$ and the three local η-spinon operators $\tilde{s}^l_{j,\eta}$ are particular cases of general $SU(2)$ local ηs quasi-spin operators $\tilde{q}^l_j$. The latter operators refer to all lattice sites and are associated with a general quasi-spin $SU(2)$ symmetry. The ηs quasi-spin operators $\tilde{q}^\pm_j = \tilde{q}^{x_1}_j \pm i\tilde{q}^{x_2}_j$ and $\tilde{q}^{x_3}_j$, where x_1, x_2, x_3 denotes the Cartesian coordinates, have the following expressions in terms of rotated-electron operators,

$$\begin{aligned}
\tilde{q}^-_j &= (\tilde{c}^\dagger_{j,\uparrow} + (-1)^j \tilde{c}_{j,\uparrow}) \tilde{c}_{j,\downarrow}, \\
\tilde{q}^+_j &= (\tilde{q}^-_j)^\dagger; \quad \tilde{q}^{x_3}_j = (\tilde{n}_{j,\downarrow} - 1/2).
\end{aligned} \tag{66}$$

Except for unimportant phase factors, the unrotated operators $\hat{f}^\dagger_{j,c} = \tilde{V} f^\dagger_{j,c} \tilde{V}^\dagger$, $\hat{f}_{j,c} = \tilde{V} f_{j,c} \tilde{V}^\dagger$, $\hat{q}^\pm_j = \tilde{V} \tilde{q}^\pm_j \tilde{V}^\dagger$, and $\hat{q}^{x_3}_j = \tilde{V} \tilde{q}^{x_3}_j \tilde{V}^\dagger$ corresponding to those defined in Eqs. (61) and (66) are those previously considered in Refs. [46–48]. The same applies to the related three local spin operators $\hat{s}^l_{j,s}$ and three local η-spin operators $\hat{s}^l_{j,\eta}$ given in Eq. (42). Hence again except for unimportant phase factors, in the $u \gg 1$ limit the operators defined in Eqs. (42), (61), and (66) become those of Refs. [46–48]. The advantage of our representation is that it is valid for the whole interaction range $u > 0$ rather than only in the $u \gg 1$ limit.

It is convenient to express the local operators $\tilde{s}_{j,c}$, $\tilde{s}^h_{j,c}$, and $\tilde{s}^l_{j,\alpha}$ where $l = \pm, x_3$ and $\alpha = s, \eta$ as,

$$\begin{aligned}
\tilde{s}_{j,c} &= n_{j,c}; \quad \tilde{s}^h_{j,c} = (1 - n_{j,c}), \\
\tilde{s}^l_{j,s} &= n_{j,c} \tilde{q}^l_j; \quad \tilde{s}^l_{j,\eta} = (1 - n_{j,c}) \tilde{q}^l_j, \quad l = \pm, x_3.
\end{aligned} \tag{67}$$

Here $n_{j,c}$ is the c fermion local density operator given in Eq. (62). Hence the ηs quasi-spin operators $\tilde{q}^l_j$ is given by,

$$\tilde{q}^l_j = \tilde{s}^l_{j,s} + \tilde{s}^l_{j,\eta}, \quad l = \pm, x_3. \tag{68}$$

The expressions provided in the above equations are consistent with the spin $SU(2)$ and η-spin $SU(2)$ symmetries being particular cases of the quasi-spin $SU(2)$ symmetry. Within them that the three local spinon operators $\tilde{s}^l_{j,s}$ and three local η-spinon operators $\tilde{s}^l_{j,\eta}$ are associated with $SU(2)$ algebra representations defined in two independent sets of sites, (i) the $2S_c$ spin-up and spin-down rotated-electron singly occupied sites and (ii) the $2S^h_c$ rotated-electron doubly-occupied and unoccupied sites, respectively, is made explicit. The c fermion and c fermion hole local density operators $n_{j,c}$ and $(1 - n_{j,c})$ in the expressions of the operators $\tilde{s}^l_{j,s}$ and $\tilde{s}^l_{j,\eta}$ provided in Eq. (67) play the role of projectors onto such two sets of lattice-site rotated-electron occupancies, respectively.

The c fermion operators and ηs quasi-spin operators given in Eqs. (61) and (67) and the related spinon and η-spinon operators defined in terms of the local c fermion number operators and ηs quasi-spin operators in Eq. (66) are mapped from the rotated-electron operators by an exact local transformation that does not introduce constraints. Given their direct relation to the generators of the model global symmetry, their occupancy configurations naturally generate representations of the corresponding global symmetry algebra. Consistent, inversion of the relations without constraints given in Eqs. (61) and (66) leads to,

$$\begin{aligned}
\tilde{c}^\dagger_{j,\uparrow} &= f^\dagger_{j,c} \left(\frac{1}{2} - \tilde{q}^{x_3}_j\right) + (-1)^j f_{j,c} \left(\frac{1}{2} + \tilde{q}^{x_3}_j\right), \\
\tilde{c}^\dagger_{j,\downarrow} &= (f^\dagger_{j,c} + (-1)^j f_{j,c}) \tilde{q}^+_j, \\
\tilde{c}_{j,\uparrow} &= f_{j,c} \left(\frac{1}{2} - \tilde{q}^{x_3}_j\right) + (-1)^j f^\dagger_{j,c} \left(\frac{1}{2} + \tilde{q}^{x_3}_j\right), \\
\tilde{c}_{j,\downarrow} &= (f_{j,c} + (-1)^j f^\dagger_{j,c}) \tilde{q}^-_j.
\end{aligned} \tag{69}$$

We confirm below that the c fermion operators commute with the ηs quasi-spin operators, what justifies the form of the expressions given here, whose c fermion operators position is always on the left-hand side.

In Section II B the unitary operator that relates the rotated-electron operators to electron operators was uniquely defined. This assures that also the spin-1/2 spinon, η-spin-1/2 η-spinon, and spin-less and η-spin-less c fermion operators are within our formulation defined in terms of those of the original electrons. The $M_s = 2S_c$ spin-1/2 spinons describe the spin $SU(2)$ symmetry degrees of freedom of the $2S_c$ rotated electrons that singly occupy sites. The c hidden $U(1)$ symmetry degrees of freedom of such $2S_c$ rotated electrons are described by $N_c = 2S_c$ spin-less and η-spin-less c fermions. Those carry their charge e. On the other hand, the $M_\eta = [N_a - 2S_c]$ η-spin-1/2 η-spinons describe the η-spin $SU(2)$ symmetry degrees of freedom of the $[N_a - 2S_c]$ sites doubly occupied (η-spin-projection $-1/2$ η-spinons) and unoccupied (η-spin-projection $+1/2$ η-spinons) by rotated electrons. The c hidden $U(1)$ symmetry degrees of freedom of such $[N_a - 2S_c]$ sites rotated-electron occupancies are described by $N_c^h = [N_a - 2S_c]$ spin-less and η-spin-less c fermion holes.

Consistent with the form of the rotated-electron amplitudes given in Eqs. (53) and (54), we find below that the $M_s = 2S_c$ spinons occupy a spin-effective lattice with $M_s = 2S_c$ sites and the η-spinons occupy a η-spin-effective lattice with $M_\eta = [N_a - 2S_c]$ sites. The c fermions c effective lattice is identical to the original lattice and has $N_c = 2S_c$ occupied sites and $N_c^h = [N_a - 2S_c]$ unoccupied sites. The important role played by the c hidden $U(1)$ symmetry is confirmed by the number values $M_s = N_c = 2S_c$ and $M_\eta = N_c^h = [N_a - 2S_c]$ being determined by the eigenvalue $2S_c$ of its generator.

The rotated-electron interaction operator $\tilde{V}_D = \hat{V}^\dagger \, \hat{V}_D \, \hat{V}$ of Eq. (74) and three rotated kinetic operators of Eq. (36) have the following expressions in terms of c fermion and ηs quasi-spin operators,

$$
\tilde{V}_D = \frac{1}{2} \sum_{j=1}^{N_a} \left(\frac{1}{2} - f_{j,c}^\dagger f_{j,c} \right),
$$

$$
\tilde{T}_\gamma = - \sum_{\langle j,j' \rangle} \tilde{T}_{\gamma;,j,j'}; \qquad \tilde{T}_{\gamma;j,j'} = F_{\gamma;j,j'} \, \tilde{Q}_{|\gamma|;j,j'}, \quad \gamma = 0, \pm 1. \tag{70}
$$

Here,

$$
\begin{aligned}
F_{0;j,j'} &= f_{j,c}^\dagger f_{j',c} + f_{j',c}^\dagger f_{j,c}, \\
F_{+1;j,j'} &= (-1)^j \, f_{j,c} f_{j',c}, \\
F_{-1;j,j'} &= (-1)^j \, f_{j',c}^\dagger f_{j,c}^\dagger, \\
\tilde{Q}_{|\gamma|;j,j'} &= \left(\frac{1}{2} + \tilde{q}_j^+ \tilde{q}_{j'}^- + \tilde{q}_{j'}^+ \tilde{q}_j^- + (-1)^{|\gamma|} 2 \tilde{q}_j^{x_3} \tilde{q}_{j'}^{x_3} \right), \quad |\gamma| = 0, 1.
\end{aligned} \tag{71}
$$

For finite u values, the Hamiltonian $\hat{H}_{symm}$ of Eq. (2) does not commute with the unitary operator $\hat{V} = e^{-\hat{S}}$. Hence, alike the general operator of Eq. (39), when expressed in terms of the rotated-electron creation and annihilation operators of Eq. (16), it has an infinite number of terms,

$$
\hat{H}_{symm} = \hat{V} \, \tilde{H}_{symm} \, \hat{V}^\dagger = \tilde{H}_{symm} + [\tilde{H}_{symm}, \tilde{S}] + \frac{1}{2} [[\tilde{H}_{symm}, \tilde{S}], \tilde{S}] + \dots . \tag{72}
$$

The commutator $[\tilde{H}_{symm}, \tilde{S}]$ does not vanish except for $u \to \infty$ so that $\hat{H}_{symm} \neq \tilde{H}_{symm}$ for finite values of u.

The Hubbard Hamiltonian given in Eq. (72) may be developed into an expansion whose order refers to the number of rotated kinetic operators $\tilde{T}_\gamma$, independently of their type, $\gamma = 0, \pm 1$. To fourth order it reads,

$$
\begin{aligned}
\hat{H}_{symm} &= \hat{H}^{(0)} + \hat{H}^{(1)} + \hat{H}^{(2)} + \hat{H}^{(3)} + \hat{H}^{(4)} + \dots, \\
\hat{H}^{(0)} &= U \tilde{V}_D; \qquad \hat{H}^{(1)} = t \tilde{T}_0, \\
\hat{H}^{(2)} &= -\frac{t^2}{U} \tilde{T}_{-1} \tilde{T}_{+1}, \\
\hat{H}^{(3)} &= \frac{t^3}{U^2} [\tilde{T}_{-1} \tilde{T}_0 \tilde{T}_{+1} - \frac{1}{2} (\tilde{T}_{-1} \tilde{T}_{+1} \tilde{T}_0 + \tilde{T}_0 \tilde{T}_{-1} \tilde{T}_{+1})] \\
\hat{H}^{(4)} &= \frac{t^4}{U^3} [\tilde{T}_{-1} \tilde{T}_0 \tilde{T}_{+1} \tilde{T}_0 + \tilde{T}_0 \tilde{T}_{-1} \tilde{T}_0 \tilde{T}_{+1} - \tilde{T}_{-1} \tilde{T}_0^2 \tilde{T}_{+1} - \frac{1}{2} \tilde{T}_{-1}^2 \tilde{T}_{+1}^2 \\
&\quad + \tilde{T}_{-1} \tilde{T}_{+1} \tilde{T}_{-1} \tilde{T}_{+1} - \frac{1}{2} (\tilde{T}_{-1} \tilde{T}_{+1} \tilde{T}_0^2 + \tilde{T}_0^2 \tilde{T}_{-1} \tilde{T}_{+1}) \\
&\quad + \theta \, (2 \tilde{T}_0 \tilde{T}_{-1} \tilde{T}_{+1} \tilde{T}_0 - \tilde{T}_{-1} \tilde{T}_{+1} \tilde{T}_0^2 - \tilde{T}_0^2 \tilde{T}_{-1} \tilde{T}_{+1})], \quad \theta - \text{real} - \text{number parameter}. \tag{73}
\end{aligned}
$$

This corresponding Hamiltonian expansion can be expressed in terms either of rotated-electron operators or c fermion and ηs quasi-spin operators. (The latter expression is obtained by the use of Eqs. (70) and (71).)

First, in the present 1D case the BA solution implicitly performs for the whole $u > 0$ interaction range the sum of all Hamiltonian terms on the right-hand-side of both Eqs. (72) and (73) and beyond. The resulting formal Hamiltonian expression is given in terms of c fermion operators and operators of well-defined η-spin-neutral η-spinon composite objects and spin-neutral spinon composite objects below in Section V E. The general Hamiltonian expressions provided in Eqs. (72) and (73) are valid for the Hubbard model on other lattices.

Second, in the $u \gg 1$ limit the rotated-electron creation and annihilation operators in the Hamiltonian expression provided in Eq. (73) become electron creation and annihilation operators, respectively. In the large-u limit that Hamiltonian expression for the model on the 1D lattice and other lattices was considered previously by many authors, as for instance in Refs. [38, 49, 50]. Apparently, such a Hamiltonian t/U expansion is formally similar in terms of electron operators, as given in such references, and in terms of rotated-electron operators, as provided in Eq. (73). However that is only so for very large u values. For instance, if for intermediate u values one expresses the t^2/U, t^3/U^2, and t^4/U^3 terms of the Hamiltonian given in Eq. (73) in electron creation and annihilation operators, one finds many complicated higher order t^j/U^{j-1} terms where $j > 2$, $j > 3$, and $j > 4$, respectively. Indeed for small and intermediate u values the first few terms of the Hamiltonian expression in terms of rotated-electron operators describe many higher-order electron processes.

The use of our operational representation renders the intermediate-u quantum problem in terms of rotated electrons similar to the corresponding large-u quantum problem in terms of electrons. As confirmed in later sections, the effect of decreasing u involves an increase of the energy bandwidth of an effective spin band associated with neutral two-spinon occupancy configurations. The intermediate-u rotated-electron processes may be associated with exchange constants describing rotated-electron motion touching progressively larger number of sites. Within the rotated-electron representation used here, such Hamiltonian terms emerge naturally upon decreasing the magnitude of u. For moderate u the rotated-electron operators generate a much simpler form for the energy eigenstates as well as for complicated processes involving a large number of electrons. As mentioned above, in the large-u limit the rotated-electrons become electrons, so that the usual picture of Refs. [38, 49, 50] is recovered.

We call off-diagonal terms of an operator expansion in terms of rotated-electron creation and annihilation operators as that given in Eq. (39), those that do not preserve the numbers of rotated-electron singly and doubly occupied sites. An interesting technical detail is that up to third order all the diagonal terms of the expansion provided in Eq. (73) are generated by the rotated-electron leading-order term, $-(t/U)[\tilde{T}_{+1} - \tilde{T}_{-1}]$, of the operator $\tilde{S}$. This is because when expressed in terms of electron operators the Hubbard Hamiltonian does not contain any off-diagonal terms with more than two electron operators. (In this case the off-diagonal terms refer to electron doubly occupied sites.)

For the Hamiltonian expansion in terms of rotated-electron operators (and thus of electron operators for $u \gg 1$) only the Hamiltonian terms $\hat{H}^{(0)}$, $\hat{H}^{(1)}$, $\hat{H}^{(2)}$, and $\hat{H}^{(3)}$ to third order given in Eq. (73) are universal. The form of the terms of fourth and larger order is different for each electron - rotated-electron unitary transformation. For the fourth-order term $\hat{H}^{(4)}$ given in that equation only the real-number parameter θ value is not universal, being unitary-transformation dependent [38]. For instance, the methods of Refs. [49] and [50] refer to two different large-u electron - rotated-electron unitary transformations whose θ values are $\theta = 0$ and $\theta = 1/4$, respectively. Moreover, one of the methods of Ref. [38] refers to an electron - rotated-electron unitary transformation whose θ value is $\theta = 1/2$. In this paper the value of the parameter θ associated with the specific electron - rotated-eleectron unitary transformation performed by the BA solution is not computed. Indeed, as confirmed below in Section V E, that solution performs the sum of all Hamiltonian terms on the right-hand-side of Eq. (73) and beyond, so that such a value is not needed for our studies.

Note that the rotated-electron on-site interaction operator,

$$\tilde{V}_D = \hat{V}^\dagger \hat{V}_D \hat{V} = \sum_{j=1}^{N_a} \tilde{V}_{D,j}; \quad \tilde{V}_{D,j} = (\tilde{n}_{j,\uparrow} - 1/2)(\tilde{n}_{j,\downarrow} - 1/2), \tag{74}$$

which in terms of c fermion operators has a non-interating form given in Eq. (70), appears only once in the Hamiltonian expression provided in Eq. (73). Indeed the Hamiltonian terms of order higher than zero involve only the three kinetic operators $\tilde{T}_0$, $\tilde{T}_{-1}$, and $\tilde{T}_{+1}$. This is so because the derivation of such a Hamiltonian expression relies on the systematic use of the commutator,

$$[\tilde{V}_D, \tilde{T}_\gamma] = \gamma \tilde{T}_\gamma, \quad \gamma = 0, \pm 1. \tag{75}$$

B. The elementary objects operator algebra

Since the electron - rotated-electron transformation associated with the operator $\hat{V}$ is unitary, the rotated-electron operators $\tilde{c}^{\dagger}_{j,\sigma}$ and $\tilde{c}_{j,\sigma}$ of Eq. (16) have the same anticommutation relations as the corresponding electron operators $c^{\dagger}_{j,\sigma}$ and $c_{j,\sigma}$, respectively. Similarly, the local c fermion operators of Eq. (61) and six local spinon and η-spinon operators of Eq. (64) have the same algebra as the corresponding unrotated spin-less and η-spin-less fermion operators of Eq. (57) and six local operators of Eq. (42), respectively. The former operators play a more general role in the physics of the model. The latter operators are a particular case of the former operators associated with the $u \gg 1$ limit physics. Hence for simplicity in the following we provide the algebra of the local c fermion operators of Eq. (61) and three ηs quasi-spin operators of Eq. (66). The $SU(2)$ algebra of the latter three operators fully determines that of the three local spinon operators and three local η-spinon operators of Eq. (64), respectively. Given the unitarity of the the operator $\hat{V}$, that of the corresponding unrotated local operators is similar.

Straightforward manipulations based on Eqs. (61) and (66) lead to the following algebra for the c fermion operators,

$$\{f^{\dagger}_{j,c}, f_{j',c}\} = \delta_{j,j'}; \quad \{f^{\dagger}_{j,c}, f^{\dagger}_{j',c}\} = \{f_{j,c}, f_{j',c}\} = 0 \,, \tag{76}$$

and the c fermion operators and the local ηs quasi-spin operators,

$$[f^{\dagger}_{j,c}, \tilde{q}^{l}_{j'}] = [f_{j,c}, \tilde{q}^{l}_{j'}] = [f^{\dagger}_{j,c}, \tilde{s}^{l}_{j',\alpha}] = [f_{j,c}, \tilde{s}^{l}_{j',\alpha}] = 0 \,, \quad l = \pm, x_3 \,, \quad \alpha = \eta, s \,. \tag{77}$$

The $SU(2)$ algebra obeyed by rotated local quasi-spin operators $\tilde{q}^{l}_{j}$ where $l = x_3, \pm$, such that $\tilde{q}^{\pm}_{j} = \tilde{q}^{x_1}_{j} \pm i\, \tilde{q}^{x_2}_{j}$, and corresponding η-spin ($\alpha = \eta$) and spin ($\alpha = s$) operators $\tilde{s}^{l}_{j,\alpha}$ is,

$$[\tilde{q}^{+}_{j}, \tilde{q}^{-}_{j'}] = \delta_{j,j'}\, 2\, \tilde{q}^{x_3}_{j}; \quad [\tilde{q}^{\pm}_{j}, \tilde{q}^{x_3}_{j'}] = \mp\delta_{j,j'}\, \tilde{q}^{\pm}_{j} \,, \tag{78}$$

and

$$[\tilde{s}^{+}_{j,\alpha}, \tilde{s}^{-}_{j',\alpha'}] = \delta_{j,j'}\delta_{\alpha,\alpha'}\, 2\, \tilde{s}^{x_3}_{j,\alpha}; \quad [\tilde{s}^{\pm}_{j,\alpha}, \tilde{s}^{x_3}_{j',\alpha'}] = \mp\delta_{j,j'}\delta_{\alpha,\alpha'}\, \tilde{s}^{\pm}_{j,\alpha} \,, \quad \alpha, \alpha' = \eta, s \,, \tag{79}$$

respectively. Moreover, one has that $[\tilde{q}^{l}_{j}, \tilde{q}^{l}_{j'}] = 0$ and $[\tilde{s}^{l}_{j,\alpha}, \tilde{s}^{l}_{j',\alpha'}] = 0$ where $l = 0, \pm$ and $\alpha, \alpha' = \eta, s$.

The c fermion and ηs quasi-spin operator algebras refer to the whole Hilbert space. On the other hand, those of the η-spinon and spinon operators correspond to well-defined subspaces spanned by states whose value of the number $2S_c$ of rotated-electron singly occupied sites is fixed. This assures that the value of the corresponding η-spinon number $M_{\eta} = [N_a - 2S_c]$ and spinon number $M_s = 2S_c$ is fixed as well.

IV. THREE EFFECTIVE LATTICES AND THE SPINON AND η-SPINON TRANSFORMATION LAWS

Here we introduce three effective lattices associated with our operator formulation. Furthermore, we investigate the consequences of the spinon and η-spinon transformation laws under the electron - rotated-electron unitary transformation.

A. Three effective lattices

Within the present operator formulation, the rotated-electron occupancy configurations that generate the 4^{N_a} energy eigenstates have three degrees of freedom associated with the functions $\phi^{c}_{U(1)}(x^{s}_1, ..., x^{s}_{N^{s}_R})$, $\phi^{\eta}_{SU(2)}(x^{d}_1, x^{d}_2, ..., x^{d}_{N^{\eta,0}_{R,-1/2}})$, and $\phi^{s}_{SU(2)}(x^{s\downarrow}_1, ..., x^{s\downarrow}_{N^{s,0}_{R,-1/2}})$, respectively, in the rotated-electron amplitude general expression of Eqs. (53) and (54). Such rotated-electron occupancy configurations three degrees of freedom are within that formulation naturally described in terms of independent occupancy configurations of c fermions, η-spinons, and spinons, respectively. (The relationship of the operators of the c fermions to those of the rotated electrons is provided in Eq. (61). That of the operators of the η-spinons and spinons to the rotated-electron operators is given in Eqs. (66)-(67).)

The direct relation in the $u \to \infty$ limit of the rotated-electron amplitudes given in Eqs. (53) and (54) to those of the electrons derived in Ref. [40] was clarified in Section II B. We have found that in such rotated-electron amplitudes the spatial coordinates $x^{s}_1, ..., x^{s}_{N^{s}_R}$ refer to the rotated-electron singly occupied sites in the original lattice. Within our formulation, they correspond to the spatial coordinates $x_1, ..., x_{N_c}$ of the $N_c = 2S_c$ c fermions in their c effective

lattice with N_a sites. Moreover, the spatial coordinates $x_1^d, ..., x_{N_{R,-1/2}^{\eta,0}}^d$ in such amplitudes correspond to the rotated-electron doubly occupied sites that are not generated from η-spin-flip processes in an effective lattice containing only the rotated-electron doubly and unoccupied sites. Within our formulation they are found below to refer to the spatial coordinates $x_1, ..., x_{M_{\eta,-1/2}^{bo}}$ of $M_{\eta,-1/2}^{bo} = [N_a - 2S_c - 2S_\eta]/2$ *anti-bound* η-spinons of η-spin projection $-1/2$ in the η-spin effective lattice with $M_\eta = [N_a - 2S_c]$ sites. Indeed, the rotated-electron amplitudes of Eqs. (53) and (54) are independent of the spatial coordinates of the n_η rotated-electron doubly occupied sites that are generated from η-spin-flip processes. Those are found below to correspond to the $M_{\eta,-1/2}^{un} = n_\eta$ *unbound* η-spinons of η-spin projection $-1/2$, which are invariant under the electron - rotated-electron unitary transformation. Finally, the spatial coordinates $x_1^{s\downarrow}, ..., x_{N_{R,-1/2}^{s,0}}^{s\downarrow}$ refer to the down spins that are not generated from spin-flip processes in an effective lattice containing only rotated-electron singly occupied sites. They are found below to correspond to the spatial coordinates $x_1, ..., x_{M_{s,-1/2}^{bo}}$ of $M_{s,-1/2}^{bo} = [S_c - S_s]$ *bound* spinons of spin projection $-1/2$ in the spin effective lattice with $M_s = 2S_c$ sites. Again, the rotated-electron amplitudes are independent of the spatial coordinates of the n_s down spins of rotated-electron singly occupied sites that are generated by spin-flip processes. Those are found below to correspond to the $M_{s,-1/2}^{un} = n_s$ *unbound* spinons of spin projection $-1/2$, which are invariant under the electron - rotated-electron unitary transformation.

For the Bethe states the numbers given in Eq. (7) vanish, $n_\eta = n_s = 0$. Thus all unbound η-spinons in such states have η-spin projection $+1/2$ and all unbound spinons have spin projection $+1/2$. This is equivalent to the absence of both rotated-electron doubly occupied sites generated from η-spin-flip processes and down spins of rotated-electron singly occupied sites generated from spin-flip processes.

The site order invariance occurring in the 1D Hubbard model plays an important role in the occupancy configurations order of the sites of the spin, η-spin, and c effective lattices. The occupancies of the sites of the spin effective lattice correspond to the spin degrees of freedom of those singly occupied by rotated electrons in the original lattice. A given spinon occupancy configuration of that effective lattice refers to the order of the spins of such rotated electrons, independently of the positions in the original lattice of the sites unoccupied and doubly occupied by rotated electrons. Similarly, the occupancies of the sites of the η-spin effective lattice correspond to the η-spin degrees of freedom of those unoccupied and doubly occupied by rotated electrons in the original lattice. A given η-spinon occupancy configuration of such an effective lattice corresponds to the order of the rotated-electron unoccupied and doubly occupied sites, independently of the positions in the original lattice of the sites singly occupied by rotated electrons.

Consistent, neither the spinon distribution of the functions $\phi_{SU(2)}^s(x_1^{s\downarrow}, ..., x_{N_{R,-1/2}^{s,0}}^{s\downarrow})$ nor the η-spinon distribution associated with the relative distribution of the rotated-electron unoccupied and doubly occupied sites of the functions $\phi_{SU(2)}^\eta(x_1^d, x_2^d, ..., x_{N_{R,-1/2}^{\eta,0}}^d)$ do change if the chain of rotated-electron singly occupied sites is "diluted" by rotated-electron unoccupied and doubly occupied sites, making possible also direct propagation for the rotated electrons. Such a propagation is described by independent occupancy configurations associated with the c fermion distribution of the function $\phi_{U(1)}^c(x_1^s, ..., x_{N_R^s}^s)$. This important property of the rotated-electron amplitudes of Eqs. (53) and (54) is behind the independence of the c effective lattice, η-spin effective lattice, and spin effective lattice occupancy configurations.

Except for $u \gg 1$, such an independence of the rotated-electron occupancy configurations three degrees of freedom is lost if one uses descriptions based on electrons rather than rotated electrons, as defined in Section II B. The c effective lattice is identical to the original lattice. Its sites are then labelled by the index $j = 1, ..., N_a$. For subspaces with fixed $2S_c$ values, the representations of the c hidden $U(1)$ symmetry algebra in the model global symmetry algebra are generated by $C_{N_a}^{N_c}$ independent occupancy configurations of the $N_c = 2S_c$ c effective lattice occupied sites relative to its $N_c^h = [N_a - 2S_c]$ unoccupied sites. Here and throughout this paper the symbol $C_{N_a}^{N_c}$ refers to the usual mathematical formula,

$$C_{N_a}^{N_c} = \binom{N_a}{N_c} = \frac{N_a!}{N_c!(N_a - N_c)!}, \quad N_a \geq N_c.$$

For a given energy eigenstate, the c fermion $N_c = 2S_c$ occupied and $N_c^h = [N_a - 2S_c]$ unoccupied sites have the same spatial coordinates as the $N_R^s = 2S_c$ sites singly occupied by rotated electrons and the $N_R^\eta = [N_a - 2S_c]$ sites doubly occupied and unoccupied by rotated electrons, respectively. Hence $C_{N_a}^{2S_c} = C_{N_a}^{N_c} = C_{N_a}^{N_c^h}$. The c effective lattice occupancy configurations and corresponding c hidden $U(1)$ symmetry algebra representations are insensitive to which of the original lattice $N_R^s = 2S_c$ sites are singly occupied by spin-up or spin-down rotated electrons and which of that lattice $N_R^\eta = [N_a - 2S_c]$ sites are doubly occupied or unoccupied by rotated electrons. As found below, representations of the c hidden $U(1)$ symmetry algebra may alternatively be generated by corresponding c band discrete momentum value occupancy configurations associated with the c fermion operators defined in Eq. (63).

The spinon and η-spinon distributions over the above-mentioned two sets of $N_R^s = 2S_c$ and $N_R^\eta = [N_a - 2S_c]$ sites of the original lattice, respectively, generate the spin $SU(2)$ algebra and η-spin $SU(2)$ algebra representations. Those correspond to the spin and η-spin degrees of freedom of independent rotated-electron occupancy configurations of the sets of $N_R^s = 2S_c$ sites and $N_R^\eta = [N_a - 2S_c]$ sites, respectively, of the original lattice. Consistent, the $M_s = N_R^s = 2S_c$ spinons only "see" the $N_R^s = 2S_c$ sites singly occupied by rotated electrons. The $M_\eta = N_R^\eta = [N_a - 2S_c]$ η-spinons only "see" the $N_R^\eta = [N_a - 2S_c]$ sites doubly occupied and unoccupied by rotated electrons. The role of the corresponding $C_{N_a}^{N_c} = C_{N_a}^{N_c^h}$ c fermion occupancy configurations is to store the information on the positions in the original lattice of the $N_R^s = 2S_c$ sites singly occupied by rotated electrons relative to the $N_R^\eta = [N_a - 2S_c]$ sites doubly occupied and unoccupied by rotated electrons.

This is consistent with the spinon and η-spinon distributions being independent. The distributions of $M_\eta = N_R^\eta = [N_a - 2S_c]$ η-spinons and $M_s = N_R^s = 2S_c$ spinons use the sets of $N_R^\eta = [N_a - 2S_c]$ rotated-electron doubly occupied plus unoccupied sites and $N_R^s = 2S_c$ rotated-electron singly occupied sites as independent η-spin and spin effective lattices, respectively. The number of sites of such effective lattices are in this paper often denoted by N_{a_η} and N_{a_s}, respectively. They read,

$$N_{a_\eta} = M_\eta = N_R^\eta = [N_a - 2S_c]; \quad N_{a_s} = M_s = N_R^s = 2S_c, \tag{80}$$

and obey the sum-rule $N_a = [N_{a_\eta} + N_{a_s}]$. The η-spinon occupancy configurations refer to the operators $\tilde{s}_{j,\eta}^l$ of Eq. (67), which act only onto the $N_{a_\eta} = N_R^\eta = [N_a - 2S_c]$ sites of the η-spin effective lattice. As discussed in Section III A, the spinon occupancy configurations correspond to the operators $\tilde{s}_{j,s}^l$ given in the same equation, which act onto the $N_{a_s} = N_R^s = 2S_c$ sites of the spin effective lattice. This is assured by the operators $(1 - n_{j,c})$ and $n_{j,c}$ in their expressions provided in that equation, which play the role of projectors onto the η-spin and spin effective lattice, respectively.

Within the present $N_a \gg 1$ limit, the spin effective lattice spacing a_s and η-spin effective lattice spacing a_η refers to the average spacing between the c effective lattice occupied sites and between such a lattice unoccupied sites, respectively,

$$a_\alpha = \frac{L}{N_{a_\beta}} = \frac{N_a}{N_{a_\beta}} a; \quad \alpha = \eta, s. \tag{81}$$

Within that limit, the spin effective lattice spacing a_s (and η-spin effective lattice spacing a_η) is a well-defined concept for finite values of the electronic density n (and hole concentration $(1-n)$). Such spin and η-spin effective lattices obey the physical requirement condition that in the $(1-n) \to 0$ and $(1-n) \to \pm 1$ limit, respectively, they equal the original lattice. Indeed, in the $(1-n) \to 0$ (and $(1-n) \to \pm 1$) limit one has that $N_{a_s} = N_a$ and the η-spin effective lattice (and $N_{a_\eta} = N_a$ and the spin effective lattice) does not exist. Consistent with the expression $a_\alpha = L/N_{a_\beta} = [N_a/N_{a_\beta}]a$ of Eq. (81) where $\alpha = \eta, s$, the η-spin (and spin) effective lattice has the same length as the original lattice. The number of sites sum-rule $[N_{a_\eta} + N_{a_s}] = N_a$ holds. Thus the η-spin and spin effective lattices have in general a number of sites N_{a_η} and N_{a_s}, respectively, smaller than that of the original lattice, N_a. Their lattice spacings provided in Eq. (81) are in general larger than that of the original lattice.

We recall that the present spinon description is normal-ordered relative to the $S_\eta = N_a/2; S_s = 0; 2S_c = 0$ electron and rotated-electron vacuum in that such state is not populated by spinons. For it the number of η-spinons is maximum and given by N_a. Consistent, for it the spin effective lattice does not exist whereas the η-spin effective lattice is identical to the original lattice. Note that the $S_\eta = N_a/2; S_s = 0; 2S_c = 0$ electron and rotated-electron vacuum is the η-spin LWS of a multiplet tower of $N_a + 1$ states. All such states have no spinons, no c fermions, N_a η-spinons, and N_a c fermion holes. For such states electrons equal rotated electrons whose number is $N = [S_\eta + S_\eta^{x_3}] = 0, 2, 4, ..., N_a$. All such electrons refer to $N/2 = [S_\eta + S_\eta^{x_3}]/2 = 0, 1, 2, ..., N_a/2$ spin-singlet on-site pairs. On the other hand, the η-spinon description is normal-ordered relative to the $S_\eta = 0; S_s = 0; 2S_c = N_a$ absolute ground state, which is not populated by η-spinons, yet the number of spinons is maximum, reading N_a. Hence for it the η-spin effective lattice does not exist, the spin effective lattice being identical to the original lattice.

We denote the one-site states that describe the rotated-electron on-site occupancies by $|j, l_{SU(2)}, l_c\rangle$. Here $j = 1, ..., N_a$ is the site index of the rotated-electron original lattice. The four values of the index $l_{SU(2)} = \odot, \uparrow\downarrow, \uparrow, \downarrow$ refer to the four rotated-electron occupancies associated with the ηs quasi-spin $SU(2)$ symmetry degrees of freedom. Those separate into two types of occupancies: (i) The occupancies of the η-spin effective lattice $N_{a_\eta} = N_R^\eta = [N_a - 2S_c]$ sites associated with the η-spin $SU(2)$ symmetry degrees of freedom; (ii) Those of the spin effective lattice $N_{a_s} = N_R^s = 2S_c$ sites associated with the spin $SU(2)$ symmetry degrees of freedom. Each on-site occupancy is described by the $+1/2$ η-spinon ($l_{SU(2)} = \odot$) and $-1/2$ η-spinon ($l_{SU(2)} = \uparrow\downarrow$) and the $+1/2$ spinon ($l_{SU(2)} = \uparrow$) and $-1/2$ η-spinon ($l_{SU(2)} = \downarrow$), respectively. The two index values $l_c = h_c$ and $l_c = p_c$ correspond to c effective lattice on-site occupancies. They refer to a c fermion unoccupied site and occupied site, respectively. Such c fermion occupancies are associated with the c

hidden $U(1)$ symmetry degrees of freedom of the corresponding on-site rotated-electron occupancies. Hence $l_c = h_c$ for $l_{SU(2)} = \odot, \uparrow\downarrow$ and $l_c = p_c$ for $l_{SU(2)} = \uparrow, \downarrow$.

As given in the second expression of Eq. (50), any of the 4^{N_a} energy eigenstates $|\Psi_{l_o, l_\triangle, u}\rangle$ may be expressed as a superposition of a sub-set of states $|u; x_1^s, ..., x_{N_R^s}^s; x_1^d, ..., x_{N_{R,-1/2}^{\eta,0}}^d; x_1^{s\downarrow}, ..., x_{N_{R,-1/2}^{s,0}}^{s\downarrow}\rangle$ describing local rotated-electron occupancy configurations. The latter states may be rewritten in terms of spinon, η-spinon, and c fermion occupancy configurations as,

$$|\Psi_{loc}\rangle = \prod_{j=1}^{N_a} |j, l_{SU(2)}(j), l_c(j)\rangle. \tag{82}$$

Each of such subsets contains all states of the form provided in Eq. (82) with the same numbers of sites singly occupied by spin-up rotated electrons, singly occupied by spin-down rotated electrons, unoccupied by rotated electrons, and doubly occupied by rotated electrons. (The site variable $j = 1, ..., N_a$ in the argument of the indices $l_{SU(2)}(j) = \odot, \uparrow\downarrow, \uparrow, \downarrow$ and $l_c(j) = h_c, p_c$ of the local-rotated-electron states given in Eq. (82) accounts of course for their values dependence on the on-site index j.)

Analysis of the expressions provided in Eq. (61) reveals that upon acting onto the one-site states $|j, l_{SU(2)}, h_c\rangle$ (and $|j, l_{SU(2)}, p_c\rangle$), in addition to creating (and annihilating) one c fermion, a c fermion operator $f_{j,c}^\dagger$ (and $f_{j,c}$) removes one site from the η-spin (and spin) effective lattice and adds one lattice to the spin (and η-spin) effective lattice as follows,

$$f_{j,c}^\dagger |j, \odot, h_c\rangle = |j, \uparrow, p_c\rangle; \quad f_{j,c}^\dagger |j, \uparrow\downarrow, h_c\rangle = (-1)^j |j, \downarrow, p_c\rangle,$$
$$f_{j,c} |j, \uparrow, p_c\rangle = |j, \odot, h_c\rangle; \quad f_{j,c} |j, \downarrow, p_c\rangle = (-1)^j |j, \uparrow\downarrow, h_c\rangle. \tag{83}$$

The spin and η-spin effective lattices are thus exotic. The number of their sites, $N_{a_s} = 2S_c$ and $N_{a_\eta} = 2S_c^h$, respectively, varies by ± 1 and ∓ 1 upon creation/annihilation of one c fermion. This is why the η-spinon and spinon operator algebras refer to subspaces spanned by energy eigenstates with fixed $2S_c$ values and thus well-defined η-spin and spin effective lattice site numbers, $N_{a_\eta} = 2S_c^h = [N_a - 2S_c]$ and $N_{a_s} = 2S_c$, respectively.

On the other hand, upon acting onto the one-site states $|j, l_{SU(2)}, l_c\rangle$, the ηs quasi-spin operators of Eq. (66) do not affect the c fermion occupancy. Thus they preserve the number of sites of both the spin and η-spin effective lattices and transform such states as follows,

$$\tilde{q}_j^+ |j, \odot, h_c\rangle = \tilde{s}_{j,\eta}^+ |j, \odot, h_c\rangle = (-1)^j |j, \uparrow\downarrow, h_c\rangle,$$
$$\tilde{q}_j^{x_3} |j, \odot, h_c\rangle = \tilde{s}_{j,\eta}^{x_3} |j, \odot, h_c\rangle = -\frac{1}{2} |j, \odot, h_c\rangle,$$
$$\tilde{q}_j^- |j, \uparrow\downarrow, h_c\rangle = \tilde{s}_{j,\eta}^- |j, \uparrow\downarrow, h_c\rangle = (-1)^j |j, \odot, h_c\rangle,$$
$$\tilde{q}_j^{x_3} |j, \uparrow\downarrow, h_c\rangle = \tilde{s}_{j,\eta}^{x_3} |j, \uparrow\downarrow, h_c\rangle = \frac{1}{2} |j, \uparrow\downarrow, h_c\rangle,$$
$$\tilde{q}_j^+ |j, \uparrow, p_c\rangle = \tilde{s}_{j,s}^+ |j, \uparrow, p_c\rangle = |j, \downarrow, p_c\rangle,$$
$$\tilde{q}_j^{x_3} |j, \uparrow, p_c\rangle = \tilde{s}_{j,s}^{x_3} |j, \uparrow, p_c\rangle = -\frac{1}{2} |j, \uparrow, p_c\rangle,$$
$$\tilde{q}_j^- |j, \downarrow, p_c\rangle = \tilde{s}_{j,s}^- |j, \downarrow, p_c\rangle = |j, \uparrow, p_c\rangle,$$
$$\tilde{q}_j^{x_3} |j, \downarrow, p_c\rangle = \tilde{s}_{j,s}^{x_3} |j, \downarrow, p_c\rangle = \frac{1}{2} |j, \downarrow, p_c\rangle. \tag{84}$$

For simplicity, in Eqs. (83) and (84) we have not included the one-site state transformations that give zero.

The result of the application onto any of the initial one-site states $|j, \odot, h_c\rangle$, $|j, \uparrow\downarrow, h_c\rangle$, $|j, \uparrow, p_c\rangle$, and $|j, \downarrow, p_c\rangle$ of the four rotated-electron operators given in Eq. (69) is a trivial problem in terms of the fermionic rotated-electron operator algebra. In Appendix A it is confirmed that the application onto such states of the operational expressions of the four rotated-electron operators in terms of ηs quasi-spin operators and c fermion operators provided in Eq. (69) leads to the same results. This confirms the faithful character of the c fermion representation and η-spinon and spinon representations associated with the ηs quasi-spin algebra.

B.   Consequences of the spinon and η-spinon transformation laws

Here we confirm that the transformation laws under the electron - rotated-electron unitary transformation of the η-spinons (and spinons) as defined in this paper contain important physical information.

1. Unbound η-spinons and unbound spinons

A well-defined number of η-spinons (and spinons) remains invariant under that unitary transformation. Since analysis of the interplay of the model global symmetry algebra representations with the BA solution reveals that they remain unbound, we call them unbound $\pm 1/2$ η-spinons (and unbound $\pm 1/2$ spinons). The invariance of the unbound η-spinons (and unbound spinons) stems from the off diagonal generators of the η-spin (and spin) algebra, which flip their η-spin (and spin), commuting with the unitary operator $\hat{V}$. This is why such generators have for $u > 0$ the same expressions in terms of electron and rotated-electron operators, as given in Eq. (41). Consistent with that invariance, the results of Ref. [22] confirm that creation of one unbound $-1/2$ η-spinon (and one unbound $-1/2$ spinon) onto a LWS ground state leads to an increase of one in the number of lattice sites doubly occupied by both electrons and rotated electrons (and singly occupied by both spin-down electrons and spin-down rotated electrons). (Within the notation of that reference, unbound $-1/2$ η-spinons and unbound $-1/2$ spinons are called $-1/2$ Yang holons and $-1/2$ HL spinons, respectively.)

The values of the numbers $M^{un}_{\eta,\pm 1/2}$ of unbound $\pm 1/2$ η-spinons and $M^{un}_{s,\pm 1/2}$ of unbound $\pm 1/2$ spinons are fully controlled by the η-spin S_η and η-spin projection $S^{x_3}_\eta = -\frac{x}{2} N_a$ and spin S_s and spin projection $S^{x_3}_s = -\frac{m}{2} N_a$, respectively, of the subspace or state under consideration as follows,

$$M^{un}_\alpha = [M^{un}_{\alpha,-1/2} + M^{un}_{\alpha,+1/2}] = 2S_\alpha; \quad M^{un}_{\alpha,\pm 1/2} = [S_\alpha \mp S^{x_3}_\alpha]; \quad \alpha = \eta, s. \tag{85}$$

Thus the η-spin S_η, η-spin projection $S^{x_3}_\eta = -\frac{x}{2} N_a$, spin S_s, and spin projection $S^{x_3}_s = -\frac{m}{2} N_a$ of an energy eigenstate are fully determined by the η-unbound spinons and unbound spinons occupancies.

For Bethe states with finite spin S_s and/or η-spin S_η all unbound spinons and/or unbound η-spinons have spin up and η-spin up, respectively. Application of the off-diagonal generators of the η-spin ($\alpha = \eta$) or spin ($\alpha = s$) algebra provided in Eq. (41) onto such $S_\alpha > 0$ states, flips the η-spin ($\alpha = \eta$) or spin ($\alpha = s$) of the unbound η-spinons or unbound spinons, respectively. The $2S_s$ and $2S_\eta$ different occupancies of the unbound spinons and unbound η-spinons, respectively, originated by such flip processes generate energy eigenstates outside the BA solution subspace.

The above invariance means that the η-spin ($\alpha = \eta$) or spin ($\alpha = s$) degrees of freedom of the rotated-electron occupancy configurations over a set of $2S_\alpha$ sites out of the whole set of N_{a_β} sites have for $u > 0$ the same form in terms of electrons and rotated electrons. On the other hand, for finite values of u the corresponding c hidden $U(1)$ symmetry degrees of freedom of such rotated-electron occupancy configurations are not in general invariant under the electron - rotated-electron unitary transformation. Such configurations are described by the c fermion occupancy configurations. The only exception is for spin fully polarized states. For those the on-site interaction does not play any role.

The invariance of the η-spin degrees of freedom of the above rotated-electron occupancy configurations implies that in each symmetry algebra representation there are exactly $2S_\eta = [M^{un}_{\eta,-1/2} + M^{un}_{\eta,+1/2}]$ sites such that $M^{un}_{\eta,-1/2}$ sites are doubly occupied and $M^{un}_{\eta,+1/2}$ sites are unoccupied both by electrons and rotated electrons. Furthermore, the invariance of the spin degrees of freedom of the sites singly occupied by rotated electrons implies that there are exactly $2S_s = [M^{un}_{s,-1/2} + M^{un}_{s,+1/2}]$ sites of the original lattice such that $M^{un}_{s,-1/2}$ sites are singly occupied both for spin-down electrons and spin-down rotated electrons and $M^{un}_{s,+1/2}$ sites are singly occupied both for spin-up electrons and spin-up rotated electrons. Consistent, it is confirmed below that symmetry implies the number $[N_{a_s} - 2S_s] = [2S_c - 2S_s]$ of sites of the spin effective lattice left over to be even and to refer to spin-singlet spinon occupancy configurations. Similarly, the number $[N_{a_\eta} - 2S_\eta] = [N_a - 2S_c - 2S_\eta]$ of sites of the η-spin effective lattice left over is even and corresponds to η-spin-singlet η-spinon occupancy configurations.

2. Anti-bound η-spinons and bound spinons

The rotated-electron occupancy configurations of the $[M^{bo}_\eta + M^{bo}_s] = [N_a - 2S_\eta - 2S_s]$ original-lattice sites left over are not invariant under the electron - rotated-electron unitary transformation. Indeed except in the $u \to \infty$ limit, the occupancy-configuration η-spin degrees of freedom of $M^{bo}_\eta = [N_a - 2S_c - 2S_\eta]$ such sites and the spin degrees of freedom of the remaining $M^{bo}_s = [2S_c - 2S_s]$ sites are different in terms of rotated electrons and electrons, respectively. (The index bo used here in the site numbers M^{bo}_η and M^{bo}_s refers to *bound*, yet such numbers are shown below in Section V G to refer to anti-bound η-spinons and bound spinons, respectively.)

Straightforward symmetry arguments given below reveal that both for rotated electrons and electrons these two sets of $M^{bo}_\eta = [N_a - 2S_c - 2S_\eta]$ and $M^{bo}_s = [2S_c - 2S_s]$ sites refer to η-spin-singlet and spin-singlet occupancy configurations, respectively. However, for finite u values such occupancy configurations preserve and do not preserve single and double occupancy for rotated electrons and electrons, respectively. The occupancy configurations of the

above remaining two sets of $M_\eta^{un} = 2S_\eta$ and $M_s^{un} = 2S_s$ sites do preserve it both for rotated electrons and electrons. Thus that for finite u values electron double and single occupancy are not good quantum numbers results only from the occupancy configurations of $[M_\eta^{bo} + M_s^{bo}] = [N_a - 2S_\eta - 2S_s]$ sites out of N_a sites. This is an important physical information brought about by the present operator formulation, which makes explicit the model global symmetry.

The above site numbers,

$$
\begin{aligned}
M_\eta^{bo} &= [N_{a_\eta} - 2S_\eta] = [N_a - 2S_c - 2S_\eta], \\
M_s^{bo} &= [N_{a_s} - 2S_s] = [2S_c - 2S_s],
\end{aligned}
\tag{86}
$$

are good quantum numbers. Their values are fully determined by those of the eigenvalue $2S_c$ of the global c hidden $U(1)$ symmetry generator and η-spin S_η or spin S_s, respectively. Thus M_η^{bo} and M_s^{bo} are not independent quantum numbers.

Although S_η and S_s may be integer or half-integer numbers, the $1/Z_2^2$ factor in the model global $[SU(2) \otimes SU(2) \otimes U(1)]/Z_2^2$ symmetry implies that only η-spin representations for which $[S_c + S_\eta]$ and $[S_c - S_s]$ are integer numbers are allowed. Since the energy eigenstates refer to representations of the model global symmetry, that restriction applies as well to such states. Hence those symmetry requirements are behind the numbers $M_\eta^{bo} = [N_a - 2S_c - 2S_\eta]$ and $M_s^{bo} = [2S_c - 2S_s]$ of Eq. (86) being even numbers for all the 4^{N_a} energy eingenstates that span the model Hilbert space. They then refer to even numbers of η-spin-$1/2$ η-spinons and spin-$1/2$ spinons, respectively. This is a necessary condition for the corresponding rotated-electron and electron occupancy configurations of such two sets of $M_\eta^{bo} = [N_a - 2S_c - 2S_\eta]$ and $M_s^{bo} = [2S_c - 2S_s]$ sites being η-spin neutral and spin neutral, respectively.

The η-spin S_η and spin S_s values and corresponding projection values $S_\eta^{x_3}$ and $S_s^{x_3}$ of an energy eigenstate are fully determined by the occupancy configurations of the unbound η-spinons and unbound spinons, respectively. This is consistent with the rotated-electron and electron occupancy configurations of the two sets of $M_\eta^{bo} = [N_a - 2S_c - 2S_\eta]$ and $M_s^{bo} = [2S_c - 2S_s]$ remaining sites being η-spin and spin neutral, respectively. In Section V this is found to be consistent as well with the BA quantum-numbers occupancies. For rotated electrons $M_\eta^{bo}/2 = [N_a/2 - S_c - S_\eta]$ of such sites are unoccupied and $M_\eta^{bo}/2 = [N_a/2 - S_c - S_\eta]$ sites are doubly occupied. Furthermore, $M_s^{bo}/2 = [S_c - S_s]$ sites are singly occupied by spin-up rotated electrons and $M_s^{bo}/2 = [S_c - S_s]$ sites are singly occupied by spin-down rotated electrons. On the other hand, for electrons at finite u values the occupancy configurations of the set of $[M_\eta^{bo} + M_s^{bo}] = [N_a - 2S_\eta - 2S_s]$ sites are η-spin-neutral and spin neutral, respectively, yet do not preserve single and double occupancy.

It follows from the known $SU(2)$ operator algebra that application onto $S_\alpha = 0$ states of the η-spin ($\alpha = \eta$) or spin ($\alpha = s$) off-diagonal generators provided in Eq. (41) gives zero. For such states, $N_{a_\beta} = M_\alpha = M_\alpha^{bo}$, so that there are no unbound η-spinons ($\alpha = \eta$) or unbound spinons ($\alpha = s$). On the other hand, application of these generators onto $S_\alpha > 0$ states flips the η-spin ($\alpha = \eta$) or spin ($\alpha = s$) of a unbound η-spinon or unbound spinon, respectively, but leaves invariant the rotated-electron occupancy configurations of the set of M_α^{bo} remaining sites. Such a set of M_η^{bo} (and M_s^{bo}) sites refers to η-spin-singlet (and spin-singlet) configurations. The energy eigenstates $|\Psi_{l_o, l_\triangle, u}\rangle$ outside the BA solution subspace have exactly the same anti-bound η-spinon and bound spinons configurations as the corresponding LWS $|\Psi_{l_o, l_\triangle^0, u}\rangle$ of the same $SU(2)$ towers. This is consistent with the amplitude equalities given in Eqs. (48) and (49). Due to the invariance under the electron - rotated-electron unitary transformation of the unbound η-spinon and unbound spinon, such amplitudes are not sensitive to their occupancy configurations, except for the phase factor $(-1)^{n_\eta}$ of Eqs. (48) and (49) where $n_\eta = M_{\eta, -1/2}^{un}$.

C. Unbound spinon and unbound η-spinon energies for both states inside and outside the BA solution subspace

In Appendix B the energy of the $\pm 1/2$ unbound η-spinons is derived. This is achieved by combining symmetry with the chemical potential curve $\mu = \mu(n)$ in Eq. (C1) of Appendix C being for $n \neq 1$ and in the $N_a \to \infty$ limit a smooth, monotonous, and continuous decreasing function of the electronic density n. A similar analysis concerning the energy of the $\pm 1/2$ unbound spinons can be carried out. Again it combines symmetry with the magnetization curve $2\mu_B H = 2\mu_B H(m)$ in Eq. (C6) of Appendix C being in the $N_a \to \infty$ limit a smooth, monotonous, and continuous decreasing function of the spin density m.

The derivation of the energy for creation onto a ground state of one $\pm 1/2$ unbound η-spinon or one $\pm 1/2$ unbound spinon requires the clarification of the related problem of the occupancies of that state. On the other hand, the BA solution subspace is smaller than and contained in the 1D Hubbard model full Hilbert space. Therefore, analysis of the energy spectra of the Bethe states alone is not enough to clarify the problem of the ground-state occupancies. In Appendix B the model global symmetry is combined with the BA solution to address that problem. Specifically, it is

found that ground states with electronic density $n \neq 1$ (and spin density $m \neq 0$) are LWSs and HWSs of the η-spin algebra (and spin algebra) for $n < 1$ and $n > 1$ (and for $m > 0$ and $m < 0$), respectively. Consistent, a $n = 1$ (and a $m = 0$) ground state is both a LWS and HWS of that algebra. In particular, the $\mu = 0$, $n = 1$, and $m = 0$ absolute ground state of the Hamiltonian $\hat{H}_{symm}$ of Eq. (2) is both a LWS and HWS of the two $SU(2)$ algebras. Hence it is both a η-spin and spin singlet with numbers $S_\eta = S_s = 0$ and $2S_c = N_a$. This last result is fully consistent with two exact theorems proved in Ref. [35], which hold as well for the Hubbard model on lattices other than the 1D lattice.

In Appendix B the energy $\varepsilon_{\eta,\pm 1/2}$ for creation onto a $n \neq 1$ ground state of one unbound η-spinon of η-spin projection $\pm 1/2$ is found to be,

$$\varepsilon_{\eta,\pm 1/2} = 2|\mu|; \quad \varepsilon_{\eta,\mp 1/2} = 0, \quad \text{sgn}\{(1-n)\}1 = \mp 1. \tag{87}$$

The relations given here hold both for finite spin densities in the range $m \in [0,n]$ for $n \in [0,1[$ and $m \in [0,2-n]$ for $n \in]1,2]$.

The $n = 1$ ground state has no η-spinons. Thus the derivation in Appendix B of the energy for creation onto that ground state of one unbound $\pm 1/2$ η-spinon relative to the zero-energy level of the Hamiltonian $\hat{H}$ of Eq. (1) uses a method other than that for an initial ground state with electronic density $n \neq 1$. The result obtained in that Appendix is,

$$\varepsilon_{\eta,\pm 1/2} = (\mu^0 \pm \mu) \quad \text{at} \quad n = 1 \quad \text{and} \quad \mu \in [-\mu^0, \mu^0]. \tag{88}$$

Such a unbound η-spinon energy is consistent with those provided in Eq. (87) for $n \neq 1$. This is confirmed upon changing the chemical potential within its $n = 1$ range, $\mu \in (-\mu^0, \mu^0)$, in the energy expression of Eq. (88) and accounting for it being given by $\mu = \mu^0$ for $n = 1^+$ and $\mu = -\mu^0$ for $n = 1^-$.

A similar analysis to that of Appendix B involving the spin $SU(2)$ algebra leads to the following energies for creation of one $\pm 1/2$ unbound spinon onto a ground state with arbitrary spin density $m \in [0,n]$ for $n \in [0,1]$ and $m \in [0,2-n]$ for $n \in [1,2]$. Relative to the zero-energy level of the Hamiltonian of Eq. (1) in a finite magnetic field H, such a $\pm 1/2$ unbound-spinon energies read,

$$\varepsilon_{s,\pm 1/2} = 2\mu_B|H|; \quad \varepsilon_{s,\mp 1/2} = 0, \quad \text{sgn}\{m\}1 = \mp 1. \tag{89}$$

The energy corresponding to a pair of unbound η-spinons of opposite η-spin projection is an important reference energy scale for our study of the energies of the anti-bound η-spinon occupancy configurations. From the energies given in Eqs. (87) and (88), one finds that relative to the zero-energy level of the Hamiltonian $\hat{H}$ of Eq. (1), such an energy scale is given by,

$$\varepsilon_{\eta,+1/2} + \varepsilon_{\eta,-1/2} = 2|\mu| \quad \text{for} \quad n \neq 1,$$
$$\varepsilon_{\eta,+1/2} + \varepsilon_{\eta,-1/2} = 2\mu^0 \quad \text{at} \quad n = 1. \tag{90}$$

Also the energy scale associated with the energy of a pair of unbound spinons of opposite spin projection plays an important role in our studies. From the energies given in Eq. (89) we find that for all spin densities and relative to the zero-energy level of the Hamiltonian $\hat{H}$ of Eq. (1), such an energy scale reads,

$$\varepsilon_{s,+1/2} + \varepsilon_{s,-1/2} = 2\mu_B|H| \quad \text{for any} \quad m. \tag{91}$$

D. The η-spinon and spinon subspace and corresponding vacuum

The numbers of $\pm 1/2$ η-spinons ($\alpha = \eta$) and $\pm 1/2$ spinons ($\alpha = s$) are fully determined by the rotated-electron numbers of Eqs. (10) and (11) as follows,

$$M_{\alpha,\pm 1/2} = N_{R,\pm 1/2}^\alpha = [M_{\alpha,\pm 1/2}^{un} + M_\alpha^{bo}/2] = [S_\alpha \mp S_\alpha^{x_3} + M_\alpha^{bo}/2] = [M_\alpha/2 \mp S_\alpha^{x_3}],$$
$$M_\alpha = N_R^\alpha = N_{a_\alpha} = [M_\alpha^{un} + M_\alpha^{bo}] = [2S_\alpha + M_\alpha^{bo}]; \quad \alpha = \eta, s. \tag{92}$$

The equalities given here do not imply that the $\pm 1/2$ η-spinons ($\alpha = \eta$) and $\pm 1/2$ spinons are the rotated-electron site occupancies with similar number values given in Eq. (10). They rather describe the η-spin and spin degrees of freedom of the rotated-electron site occupancies associated with the numbers $N_{R,\pm 1/2}^\eta$ and $N_{R,\pm 1/2}^s$, respectively. We call η-spinon and spinon subspaces those spanned by states whose value of the number $2S_c$ of rotated-electron singly occupied sites is fixed. In it the number values $N_{a_\eta} = [N_a - 2S_c]$ and $N_{a_s} = 2S_c$ of sites of the η-spin and spin effective lattices and thus $M_\eta = [N_a - 2S_c]$ and $M_s = 2S_c$ of η-spinons and spinons, respectively, are fixed as well.

Within our LWS representation, the theory vacuum of each η-spinon and spinon subspace is a η-spin and spin LWS. Its maximum spin density $m = (1 - x) = n$ is reached at a critical magnetic field $H = -H_c$, whose absolute value is defined in Eq. (C7) of Appendix C. Such a spin fully polarized state has no anti-bound η-spinons and no bound spinons, $M_\eta^{bo} = M_s^{bo} = 0$. Its electronic density is in the range $n \in [0, 1]$, so that the $2S_c$ value of that state is $2S_c = N$. It remains invariant under the electron - rotated-electron unitary transformation and reads,

$$|0_{\eta s}\rangle = |0_\eta; N_{a_\eta}\rangle \otimes |0_s; N_{a_s}\rangle \otimes |GS_c; 2S_c\rangle. \tag{93}$$

Here the η-spin $SU(2)$ vacuum $|0_\eta; N_{a_\eta}\rangle$ associated with $N_{a_\eta} = [N_a - N]$ unbound $+1/2$ η-spinons, the spin $SU(2)$ vacuum $|0_s; N_{a_s}\rangle$ with $N_{a_s} = N$ unbound $+1/2$ spinons, and the c band $U(1)$ vacuum $|GS_c; 2S_c\rangle$ with $N_c = 2S_c = N$ c fermions remain invariant under the electron - rotated-electron unitary transformation. Indeed, in this limiting case the c fermion operators are also invariant under the electron - rotated-electron unitary transformation. The above vacuum $|GS_c; 2S_c\rangle$ may be expressed as $\prod_q f_{q,c}^\dagger |GS_c; 0\rangle$.

The state $|GS_c; 0\rangle$ in $\prod_q f_{q,c}^\dagger |GS_c; 0\rangle$ is the $N_c = 2S_c = 0$ c fermion absolute vacuum. It refers to the $S_\eta = N_a/2; S_s = 0; 2S_c = 0$ electron and rotated-electron vacuum, $|0\rangle = |0_\eta; N_a\rangle \otimes |0_s; 0\rangle \otimes |GS_c; 0\rangle$. It is a limiting case of that provided in Eq. (93). It corresponds to $N_{a_\eta} = [N_a - 2S_c] = N_a$ and $N_{a_s} = 2S_c = 0$. Such a vacuum has no spin effective lattice, no spin degrees of freedom, no rotated electrons, no electrons, and no c fermions. Nonetheless within our formulation it is populated by M_η unbound η-spinons of η-spin projection $+1/2$. It is a η-spin fully polarized state with maximum hole concentration $x = (1 - n) = 1$ reached at chemical potential $\mu = -\mu^1 = -[U + 4t]/2$, Eq. (C5) of Appendix C. It has maximum η-spin value, $S_\eta = N_a/2$. The corresponding $2S_c = 0$ subspace has dimension $N_a + 1$. It is spanned by that vacuum and its $2S_c = N_a$ tower states. All such states have no spin effective lattice, no spin degrees of freedom, and no c fermions. They are populated by $N = 2n_\eta = 2M_{\eta,-1/2}^{un} = 2, 4, ..., 2N_a$ rotated electrons, which are invariant under the electron - rotated-electron unitary transformation. Hence for the $2S_c = 0$ subspace such rotated electrons are electrons.

Consistent with the c fermions one-site state transformation of Eq. (83), creation (and annihilation) of one c fermion is a process that changes the $N_c = 2S_c$ value and thus drives the system into a subspace with a different vacuum, Eq. (93). As explicitly given in that equation, such a c fermion creation (and annihilation) process involves as well addition (and removal) of one site to (and from) the spin effective lattice and removal (and addition) of one site from (and to) the η-spin effective lattice. It follows that from the point of view of the η-spin and spin degrees of freedom, c fermion creation and annihilation processes correspond to a change of quantum system. Indeed, the η-spin and spin lattices and corresponding number of sites change along with the quantum-system vacuum $|0_{\eta s}\rangle$, Eq. (93). One can then say that for the η-spinon and spinon representation there is a different quantum system for each eigenvalue $2S_c$ of the generator of the global c hidden $U(1)$ symmetry of Eqs. (43) and (65). (This is consistent with a quantum problem being defined both by a Hamiltonian and the Hilbert space its acts onto.) Specifically, the separate η-spinon and spinon operator algebra representations refer to the quantum problem described by the 1D Hubbard model in the η-spinon and spinon subspace defined above.

Finally, to illustrate the differences between the two types of occupancy configurations of unbound and bound spinons, which have finite spin S_s and are spin neutral, respectively, we consider a state $|\psi\rangle$. (Similar considerations apply to unbound and anti-unbound η-spinons.) For simplicity but without loss in generality, we consider that it belongs to a subspace whose spin effective lattice has only four sites. Hence the state has $N_c = 2S_c = 4$ c fermions, $N_c^h = [N_a - 2S_c] = [N_a - 4]$ c fermion holes, $M_s = 2S_c = 4$ spinons, and $M_\eta = [N_a - 2S_c] = [N_a - 4]$ η-spinons, where $N_a \gg 1$. Furthermore, we choose it to be a LWS with spin and spin projection $S_s = -S_s^{x_3} = 1$ and η-spin and η-spin projection $S_\eta = -S_\eta^{x_3} = [N_a - 4]/2$. Thus its numbers of unbound spinons and unbound η-spinons are $M_{s,+1/2}^{un} = [2S_c - 2S_s] = 2$, $M_{s,-1/2}^{un} = 0$ and $M_{\eta,+1/2}^{un} = [N_a - 4]$, $M_{\eta,-1/2}^{un} = 0$, respectively. Furthermore, it follows from the above number values that the state has $M_s^{un} = 2$ bound spinons and $M_\eta^{bo} = 0$ anti-bound η-spinons.

We denote by $|\psi; j = 1, 2, 3, 4\rangle$ the four-site state that describes the spin-degrees of freedom of the state $|\psi\rangle$. For simplicity, we have chosen the site index values $j = 1, 2, 3, 4$ to be those of the underlying spin effective lattice. Below we also indicate the c fermion occupancies associated with the c hidden $U(1)$ symmetry degrees of freedom of the four sites. In terms of the one-site states $|j, l_{SU(2)}(j), l_c(j)\rangle$ on the right-hand side of Eq. (82), we consider that our four-site state is given by,

$$\begin{aligned}
|\psi; j = 1, 2, 3, 4\rangle &= \frac{1}{2}[|1, \uparrow, p_c\rangle|2, \downarrow, p_c\rangle|3, \uparrow, p_c\rangle|4, \uparrow, p_c\rangle - |1, \downarrow, p_c\rangle|2, \uparrow, p_c\rangle|3, \uparrow, p_c\rangle|4, \uparrow, p_c\rangle \\
&+ |1, \uparrow, p_c\rangle|2, \uparrow, p_c\rangle|3, \uparrow, p_c\rangle|4, \downarrow, p_c\rangle - |1, \uparrow, p_c\rangle|2, \uparrow, p_c\rangle|3, \downarrow, p_c\rangle|4, \uparrow, p_c\rangle].
\end{aligned} \tag{94}$$

The identification of unbound and anti-bound spinons becomes clear if one writes such a state as a superposition of

two states. Each of them is a product of a spin-triplet two-spinon state by a spin-singlet two-spinon state,

$$
\begin{aligned}
|\psi; j = 1, 2, 3, 4\rangle &= \frac{1}{\sqrt{2}} \{ [|1, \uparrow, p_c\rangle |2, \downarrow, p_c\rangle - |1, \downarrow, p_c\rangle |2, \uparrow, p_c\rangle] \times |3, \uparrow, p_c\rangle |4, \uparrow, p_c\rangle \} \\
&+ \frac{1}{\sqrt{2}} \{ |1, \uparrow, p_c\rangle |2, \uparrow, p_c\rangle \times [|3, \uparrow, p_c\rangle |4, \downarrow, p_c\rangle - |3, \downarrow, p_c\rangle |4, \uparrow, p_c\rangle] \} .
\end{aligned}
\tag{95}
$$

The two unbound spinons are those of the spin-triplet two-spinon state. The two bound spinons are those of the spin-singlet two-spinon state.

The present $S_s^{x_3} = -1$ state $|\psi\rangle$ belongs to the subspace spanned by the Bethe states. The $S_s^{x_3} = 0$ and $S_s^{x_3} = 1$ states generated from it are outside the LWS BA solution subspace. Their corresponding four-site states,

$$
\frac{1}{2} \tilde{S}_s^\dagger |\psi; j = 1, 2, 3, 4\rangle \otimes |\psi_\eta\rangle \otimes |\psi_c\rangle ; \qquad \frac{1}{4} [\tilde{S}_s^\dagger]^2 |\psi; j = 1, 2, 3, 4\rangle \otimes |\psi_\eta\rangle \otimes |\psi_c\rangle ,
\tag{96}
$$

are given by,

$$
\begin{aligned}
\frac{1}{2} \tilde{S}_s^\dagger |\psi; j = 1, 2, 3, 4\rangle &= \frac{1}{2^{3/2}} \{ [|1, \uparrow, p_c\rangle |2, \downarrow, p_c\rangle - |1, \downarrow, p_c\rangle |2, \uparrow, p_c\rangle] \times [|3, \downarrow, p_c\rangle |4, \uparrow, p_c\rangle + |3, \uparrow, p_c\rangle |4, \downarrow, p_c\rangle] \} \\
&+ \frac{1}{2^{3/2}} \{ [|1, \downarrow, p_c\rangle |2, \uparrow, p_c\rangle + |1, \uparrow, p_c\rangle |2, \downarrow, p_c\rangle] \times [|3, \uparrow, p_c\rangle |4, \downarrow, p_c\rangle - |3, \downarrow, p_c\rangle |4, \uparrow, p_c\rangle] \} ,
\end{aligned}
\tag{97}
$$

and

$$
\begin{aligned}
\frac{1}{4} [\tilde{S}_s^\dagger]^2 |\psi; j = 1, 2, 3, 4\rangle &= \frac{1}{\sqrt{2}} \{ [|1, \uparrow, p_c\rangle |2, \downarrow, p_c\rangle - |1, \downarrow, p_c\rangle |2, \uparrow, p_c\rangle] \times |3, \downarrow, p_c\rangle |4, \downarrow, p_c\rangle \} \\
&+ \frac{1}{\sqrt{2}} \{ |1, \downarrow, p_c\rangle |2, \downarrow, p_c\rangle \times [|3, \uparrow, p_c\rangle |4, \downarrow, p_c\rangle - |3, \downarrow, p_c\rangle |4, \uparrow, p_c\rangle] \} .
\end{aligned}
\tag{98}
$$

respectively. In the above equations, $\tilde{S}_s^\dagger$ is the spin off-diagonal generator given in Eq. (41). States outside the LWS BA solution subspace differ from the corresponding states inside it only in the unbound spinons and/or unbound η-spinon occupancies. Their c fermion, spin-neutral bound spinon, and η-spin-neutral anti-bound η-spinon occupancy configurations are exactly the same.

More generally, the spin effective lattice occupancy configurations of any state with $M_s = 2S_c$ spinons and $M_s^{un} = 2S_s$ unbound spinons such that $2S_c > 2S_s$ may be written as a sum of state configurations. Each of such configurations is a product of two states: A spin-S_s M_s^{un}-spinon state and a spin-singlet M_s^{bo}-spinon state where $M_s^{un} = 2S_s$ and $M_s^{bo} = [2S_c - 2S_s]$, respectively. Alike for the simple configurations in Eqs. (95), (97), and (98), the overall spin-effective lattice state is a superposition of configuration states where the positions of the unbound spinons and anti-bound spinons is different. However, their numbers are the same in all such states.

V.   RELATION OF THE c FERMION, SPINON, AND η-SPINON OCCUPANCY CONFIGURATIONS TO THE QUANTUM NUMBERS OF THE BA SOLUTION

The counting of the independent representations of the model global symmetry algebra in its subspaces with c fermion, spinon, and η-spinon fixed numbers is used here to extract useful information on the relation of Takahasi's BA solution numbers to the objects of the present operator formulation.

A.   The thermodynamic BA equations in a notation suitable to the model global symmetry

The notations used in Ref. [1] do not account for the relation of the BA quantum numbers that label the energy eigenstates to the model global $SO(3) \otimes SO(3) \otimes U(1) = [SO(4) \otimes U(1)]/Z_2$ symmetry algebra representations. Hence here we slightly change the notations used in that paper according to such representations.

From analysis of the BA results of Ref. [1], we find that the number $M_\eta^{bo}/2$ of anti-bound η-spinon pairs considered in Section IV B is exactly the number denoted by M' in that reference. Moreover, the quantity $\sum_{n=1}^{\infty} n M_n$ appearing in Eq. (2.13d) of that paper is the number $M_s^{bo}/2$ of bound spinon pairs. It is confirmed below that the quantities denoted in Ref. [1] by M_n (and $M_n{}'$) are the number of specific types of spin-neutral spinon configurations (and η-spin-neutral η-spinon configurations) involving n bound-spinon pairs (and anti-bound-η-spinon pairs). In this paper

we denote the numbers M_n and $M_n{}'$ of that reference where $n = 1, ..., \infty$ by $N_{s\nu}$ and $N_{\eta\nu}$, where $\nu = 1, ..., \infty$, respectively. The sets of numbers $\{N_{s\nu}\}$ and $\{N_{\eta\nu}\}$ are Bethe-state good quantum numbers, which obey the sum rules $M_\alpha^{bo} = \sum_{\nu=1}^{\infty} 2\nu N_{\alpha\nu}$ for $\alpha = \eta, s$.

The BA quantum numbers whose occupancy configurations generate the Bethe states include as well those associated with the degrees of freedom of the c hidden $U(1)$ symmetry beyond $SO(4)$, in the model global $[SO(4) \otimes U(1)]/Z_2$ symmetry. Consistent with the first expression given in Eq. (B7) of Appendix B, the number of c fermions, N_c, can be written as $N_c = 2S_c = [N - M_\eta^{bo} - 2M_{\eta,-1/2}^{un}]$. For the LWS Bethe states that span the BA solution subspace one has that $2M_{\eta,-1/2}^{un} = 0$. Hence for the BA solution the N_c expression simplifies to $N_c = 2S_c = [N - M_\eta^{bo}]$. The c fermion number $N_c = 2S_c$ and thus the eigenvalue of the c hidden $U(1)$ symmetry generator, $2S_c$, appears explicitly in the BA thermodynamic equations of Ref. [1], where it is denoted by $[N - 2M']$. (Since M' is the notation of that reference for the number $M_\eta^{bo}/2$ of anti-bound η-spinon pairs, the number $[N - 2M']$ is indeed the number $N_c = 2S_c = [N - M_\eta^{bo}]$ of c fermions in the BA solution subspace.)

The thermodynamic BA equations, Eqs. (2.12a)-(2.12c) of Ref. [1], refer to subspaces spanned by Bethe states with fixed values for the set of numbers $N_c = 2S_c$ and $\{N_{\alpha\nu}\}$ where $\alpha = \eta, s$ and $\nu = 1, ..., \infty$. Such equations involve the integers or half-odd integers quantum numbers I_j, $J_\alpha'^n$, and J_α^n. (Here the index $n = 1, ..., \infty$ is that denoted in this paper by $\nu = 1, ..., \infty$.) We denote the indices α of Ref. [1], appearing in the numbers $J_\alpha'^n$ and J_α^n, by j and consider the following related quantum numbers,

$$q_j = \frac{2\pi}{N_a} I_j^c ; \quad j = 1, ..., N_a ; \qquad q_j = \frac{2\pi}{N_a} I_j^{\alpha\nu} ; \quad j = 1, ..., N_{a_{\alpha\nu}} , \tag{99}$$

where $I_j \equiv I_j^c$, $J_j'^\nu \equiv I_j^{\eta\nu}$, and $J_j^\nu \equiv I_j^{s\nu}$. The BA quantum numbers are thus those given here in units of $2\pi/N_a$. The latter are confirmed below to be discrete momentum values carried by quantum objects of our operator formulation. Although for different Bethe states one has that I_j^c, $I_j^{\eta\nu}$, and $I_j^{s\nu}$ may be integers or half-odd integers, for each such a state the corresponding discrete momentum values q_j have the usual momentum spacing, $q_{j+1} - q_j = 2\pi/N_a$.

The number values of the elementary objects whose occupancy configurations are associated with the BA solution quantum numbers and its present extension to the full Hilbert space obey the following equalities and sum rules controlled by the rotated-electron site occupancy numbers given in Eqs. (10) and (11),

$$N_c = M_s = N_R^s ; \quad N_c^h = M_\eta = N_R^\eta ,$$

$$\sum_{\nu=1}^{\infty} 2\nu N_{\alpha\nu} = N_R^\alpha - 2S_\alpha , \quad \alpha = \eta, s ,$$

$$M_{\alpha,\pm 1/2} = M_{\alpha,\pm 1/2}^{un} + \sum_{\nu=1}^{\infty} \nu N_{\alpha\nu} = N_{R,\pm 1/2}^\alpha , \quad \alpha = \eta, s . \tag{100}$$

This confirms that the BA solution accounts for the underlying rotated electrons, as defined in Section II.

The number of discrete momentum values, $N_{a_{\alpha\nu}}$, in Eq. (99) is for the BA $\alpha\nu$ band given by,

$$N_{a_{\alpha\nu}} = [N_{\alpha\nu} + N_{\alpha\nu}^h] , \quad \alpha = \eta, s , \quad \nu = 1, ..., \infty . \tag{101}$$

Here $N_{\alpha\nu}$ and $N_{\alpha\nu}^h$ are the numbers of the $\alpha\nu$ band occupied and unoccupied momentum values, respectively. From analysis of the results of Ref. [1], we find that the latter is given by,

$$N_{\alpha\nu}^h = [2S_\alpha + 2 \sum_{\nu'=\nu+1}^{\infty} (\nu' - \nu)N_{\alpha\nu'}] = [M_\alpha^{un} + 2 \sum_{\nu'=\nu+1}^{\infty} (\nu' - \nu)N_{\alpha\nu'}] , \quad \alpha = \eta, s . \tag{102}$$

Within the notation of that reference, $N_{a_{\eta\nu}}/2$ and $N_{a_{s\nu}}/2$ are the numbers on the right-hand side of the two inequalities given just above its Eq. (2.13a). The corresponding BA quantum numbers I_j^c (and $I_j^{\alpha\nu}$) where $j = 1, ..., N_a$ (and $j = 1, ..., N_{a_{\alpha\nu}}$) are integers and half-odd integers for $\sum_{\alpha\nu} N_{\alpha\nu}$ (and $[N_{a_{\alpha\nu}} - 1]$) even and odd, respectively. Furthermore, these numbers obey the inequality $|I_j^c| \leq [N_a - 1]/2$ for $\sum_{\alpha\nu} N_{\alpha\nu}$ even and $-[N_a - 2]/2 \leq I_j^c \leq N_a/2$ for $\sum_{\alpha\nu} N_{\alpha\nu}$ odd (and the inequality $|I_j^{\alpha\nu}| \leq [N_{a_{\alpha\nu}} - 1]/2$ for both $[N_{a_{\alpha\nu}} - 1]$ odd and even).

In each subspace with fixed values for the set of numbers $N_c = 2S_c$ and $\{N_{\alpha\nu}\}$ where $\alpha = \eta, s$ and $\nu = 1, ..., \infty$, the Bethe states are generated by the d_c occupancy configurations of the N_c c fermions in their c band with N_a discrete momentum values, $d_{\eta\nu}$ occupancy configurations of $N_{\eta\nu}$ filled $\eta\nu$ band discrete momentum values over the $N_{a_{\eta\nu}}$ discrete momentum values for each $\eta\nu$ branch with finite $N_{\eta\nu} > 0$ occupancy, and $d_{s\nu}$ occupancy configurations of $N_{s\nu}$ filled $\eta\nu$ band discrete momentum values over the $N_{a_{s\nu}}$ discrete momentum values for each $s\nu$ branch with finite $N_{s\nu} > 0$ occupancy. Here the dimensions d_c, $d_{\eta\nu}$, and $d_{s\nu}$ are given by,

$$d_c = C_{N_a}^{N_c} ; \quad d_{\eta\nu} = C_{N_{a_{\eta\nu}}}^{N_{\eta\nu}} ; \quad d_{s\nu} = C_{N_{a_{s\nu}}}^{N_{s\nu}} , \quad \nu = 1, ..., \infty , \tag{103}$$

respectively. It is confirmed below that the c band occupancy configurations generate representations of the c hidden $U(1)$ symmetry algebra, the set of $\eta\nu$ bands occupancy configurations generate η-spin-singlet representations of the η-spin $SU(2)$ symmetry algebra, and the set of $s\nu$ bands occupancy configurations generate spin-singlet representations of the spin $SU(2)$ symmetry algebra.

Several physical quantities may be written in functional form in terms of the c, $\eta\nu$, and $s\nu$ band distribution momentum functions $N_c(q_j)$, $N_{\eta\nu}(q_j)$, and $N_{s\nu}(q_j)$, respectively. Those are eigenvalues of number operators $\hat{N}_c(q_j)$, $\hat{N}_{\eta\nu}(q_j)$, and $\hat{N}_{s\nu}(q_j)$, respectively, whose expressions are given below in Section V E. The latter operators commute with the 1D Hubbard model Hamiltonian. The Bethe states are eigenstates of such operators. They have eigenvalues $N_\beta(q_j) = 1$ for occupied momentum values and $N_\beta(q_j) = 0$ for unoccupied momentum values where $\beta = c, \alpha\nu$, $\alpha = \eta, s$, and $\nu = 1, ..., \infty$.

That the quantum numbers q_j are the c band and $\alpha\nu$ band discrete momentum values is fully consistent with the following exact functional expression for the energy eigenstates total momentum,

$$P = \sum_{j=1}^{N_a} q_j\, N_c(q_j) + \sum_{\nu=1}^{\infty} \sum_{j=1}^{N_{a_{s\nu}}} q_j\, N_{s\nu}(q_j) + \sum_{\nu=1}^{\infty} \sum_{j=1}^{N_{a_{\eta\nu}}} [\pi - q_j]\, N_{\eta\nu}(q_j) + \pi\, M_{\eta,-1/2}\,, \qquad (104)$$

which is additive in such values. From analysis of the results of Ref. [1], one finds that for the Bethe states the momentum has the form given in Eq. (104) with $M_{\eta,-1/2} = M_\eta^{bo}/2$. By combining the BA solution with symmetry, we then straightforwardly confirm that the physical momentum expression given in that equation, where $M_{\eta,-1/2} = M_\eta^{bo}/2 + M_{\eta,-1/2}^{un}$, is valid for all energy eigenstates.

The c band discrete momentum values q_j are the conjugate variables of the c effective lattice spatial coordinates j where $j = 1, ..., N_a$. Such discrete momentum values label corresponding c fermion operators given by,

$$f_{q_j,c}^\dagger = \frac{1}{\sqrt{N_a}} \sum_{j'=1}^{N_a} e^{+i\, q_j j'}\, f_{j',c}^\dagger\,; \quad f_{q_j,c} = \left(f_{q_j,c}^\dagger\right)^\dagger\,, \qquad (105)$$

where we have used units of lattice spacing one. Consistent with the operator algebra of Eq. (76), such c fermion operators obey the following anticommutation relations,

$$\{f_{q_j,c}^\dagger, f_{q_{j'},c}\} = \delta_{j,j'}\,; \quad \{f_{q_j,c}^\dagger, f_{q_{j'},c}^\dagger\} = \{f_{q_j,c}, f_{q_{j'},c}\} = 0\,. \qquad (106)$$

Within our notation the thermodynamic BA equations, Eqs. (2.12a)-(2.12c) of Ref. [1], may be written in functional form as follows,

$$\begin{aligned}
k_c(q_j) &= q_j - \frac{2}{N_a} \sum_{\nu=1}^{\infty} \sum_{j'=1}^{N_{a_{s\nu}}} N_{s\nu}(q_{j'}) \arctan\left(\frac{\sin k_c(q_j) - \Lambda_{s\nu}(q_{j'})}{\nu u}\right) \\
&\quad - \frac{2}{N_a} \sum_{\nu=1}^{\infty} \sum_{j'=1}^{N_{a_{\eta\nu}}} N_{\eta\nu}(q_{j'}) \arctan\left(\frac{\sin k_c(q_j) - \Lambda_{\eta\nu}(q_{j'})}{\nu u}\right)\,; \quad j = 1, ..., N_a\,,
\end{aligned} \qquad (107)$$

and

$$\begin{aligned}
k_{\alpha\nu}(q_j) &= q_j - \frac{2e^{i\pi\delta_{\alpha,\eta}}}{N_a} \sum_{j'=1}^{N_a} N_c(q_{j'}) \arctan\left(\frac{\Lambda_{\alpha\nu}(q_j) - \sin k_c(q_{j'})}{\nu u}\right) \\
&\quad + \frac{1}{N_a} \sum_{\nu'=1}^{\infty} \sum_{j'=1}^{N_{a_{\alpha\nu'}}} N_{\alpha\nu'}(q_{j'}) \Theta_{\nu,\nu'}\left(\frac{\Lambda_{\alpha\nu}(q_j) - \Lambda_{\alpha\nu'}(q_{j'})}{u}\right)\,, \\
\nu &= 1, ..., \infty\,, \quad j = 1, ..., N_{a_{\alpha\nu}}\,, \quad \alpha = \eta, s\,.
\end{aligned} \qquad (108)$$

Here,

$$k_{\alpha\nu}(q_j) = \delta_{\alpha,\eta}\, 2\,\mathrm{Re}\left\{\arcsin(\Lambda_{\eta\nu}(q_j) + i\nu u)\right\}\,, \quad \nu = 1, ..., \infty\,, \quad j = 1, ..., N_{a_{\alpha\nu}}\,, \quad \alpha = \eta, s\,, \qquad (109)$$

is the $\alpha\nu$ rapidity-momentum functional. It vanishes for $\alpha = s$. The function $\Theta_{\nu,\nu'}(x)$ reads,

$$\Theta_{\nu,\nu'}(x) = \delta_{\nu,\nu'}\left\{2\arctan\left(\frac{x}{2\nu}\right) + \sum_{l=1}^{\nu-1} 4\arctan\left(\frac{x}{2l}\right)\right\} + (1 - \delta_{\nu,\nu'})\left\{2\arctan\left(\frac{x}{|\nu-\nu'|}\right)\right.$$

$$\left. + 2\arctan\left(\frac{x}{\nu+\nu'}\right) + \sum_{l=1}^{\frac{\nu+\nu'-|\nu-\nu'|}{2}-1} 4\arctan\left(\frac{x}{|\nu-\nu'|+2l}\right)\right\}. \tag{110}$$

The quantities $\Lambda_{\eta\nu,j} \equiv \Lambda_{\eta\nu}(q_j)$ (and $\Lambda_{s\nu,j} \equiv \Lambda_{s\nu}(q_j)$) are denoted in Ref. [1] by ${\Lambda'_\alpha}^n$ (and Λ_α^n) where $\alpha = j = 1, ..., N_{a_{\alpha\nu}}$ and $n = \nu = 1, ..., \infty$. Within the notation of that reference, bound states of *electron n-pairs* are described by complex numbers Λ' and *magnon bound states of n-pairs* are described by complex numbers Λ [1]. The quantities ${\Lambda'_\alpha}^n$ (and Λ_α^n) in the above equations are the real part of such complex BA rapidities.

Within the BA solution literature that followed the results of Ref. [1], the latter quantities are associated with excitations often called strings of length $n = \nu = 1, ..., \infty$ [30]. In Sections 4.2.1 and 4.2.2 of Ref. [30] those were studied for two very simple limiting states, for which electrons may be approximated by rotated electrons. In the thermodynamic limit the two electrons with opposite spin projections in the η-spin $\nu = 1$ string state considered in the former section occupy the same site. The $\nu = 1$ string involves an unoccupied site, in addition to the spin-singlet electron pair. The spin $\nu = 2$ string state considered in the latter section involves the spin degrees of freedom of the two down-spin electrons and of two out of its $N - 2$ up-spin electrons, rather than only those of the two former electrons. This is in spite of the corresponding wave functions, which are of the general form given in Eq. (19), only depending on the spatial coordinates of the spin-down and spin-up electrons and two down-spin electrons, respectively, as discussed in Section II B.

We denote by $\Lambda_{\alpha\nu}^\gamma(q_j)$ the complex BA rapidity whose real part $\Lambda_{\alpha\nu}(q_j)$ dependence on the $\alpha\nu$ bands momentum values q_j is obtained by solution of Eqs. (107)-(109). Its imaginary part is in the $N_a \rightarrow \infty$ limit independent of such momentum values. It depends solely on the on-site repulsion in units of $4t$, $u = U/4t$, and number of pairs, $\nu = 1, ..., \infty$,

$$\Lambda_{\alpha\nu}^\gamma(q_j) = \Lambda_{\alpha\nu}(q_j) + i(1 + \nu - 2\gamma)\,u\,, \quad \gamma = 1, ..., \nu\,, \quad j = 1, ..., N_{a_{\alpha\nu}}\,, \quad \nu = 1, ..., \infty\,, \quad \alpha = \eta, s\,. \tag{111}$$

For $\nu > 1$ the ν imaginary BA rapidity terms $i(1 + \nu - 2\gamma)\,u$ where $\gamma = 1, ..., \nu$ are within our operator formulation related to the attraction between the corresponding ν spin-neutral spinon pairs ($\alpha = s$) or η-spin-neutral η-spinon pairs ($\alpha = \eta$). Such ν pairs have the same momentum q_j. Except for $q_j = 0$ and $q_j = \pm q_{\alpha\nu}$, where $q_{\alpha\nu} = \pi[N_{a_{\alpha\nu}} - 1]/L$, they move coherently within the same 2ν-spinon ($\alpha = s$) or 2ν-η-spinon ($\alpha = \eta$) composite object. (At both $q_j = 0$ and $q_j = \pm q_{\alpha\nu}$ their velocity is found below to vanish.) That attraction is behind the formation of those of such composite objects that contain $\nu > 1$ pairs. Hence it is to be distinguished from the two-spinon binding and two-η-spinon anti-binding of each pair. That for $\nu = 1$ and both $\alpha = \eta, s$ the BA rapidity $\Lambda_{\alpha1}^1(q_j) = \Lambda_{\alpha1}(q_j)$ of Eq. (111) is real follows from it referring to a single pre-formed spin-neutral spinon pair ($\alpha = s$) or η-spin-neutral η-spinon pair ($\alpha = \eta$). In the second paper it is confirmed that there are no bound states of such 2ν-spinon ($\alpha = s$) or 2ν-η-spinon ($\alpha = \eta$) composite objects.

The c band and $\alpha\nu$ bands momentum values q_j appearing in Eqs. (107)-(109) and (111), which are defined in Eq. (99), are the actual quantum numbers of the BA solution. The role of the corresponding c band rapidity momentum functional $k_c(q_j)$, $\eta\nu$ band rapidity functional $\Lambda_{\eta\nu}(q_j)$, and $s\nu$ band rapidity functional $\Lambda_{s\nu}(q_j)$ is to explicit the dependence of the Bethe-states energy spectrum on such quantum numbers occupancy configurations. As confirmed below, that energy spectrum depends on the momentum occupancy configurations of the c band and $\alpha\nu$ bands through such functionals.

Combining the BA results of Ref. [1] with the model global symmetry algebra representations, one confirms that in the present $N_a \rightarrow \infty$ limit the BA solution performs a partition of the M_η^{bo}-η-spinon η-spin-singlet (and M_s^{bo}-spinon spin-singlet) configuration into a set of smaller independent η-spin-singlet (and spin-singlet) configurations. Their number is,

$$B_\alpha = \sum_{\nu=1}^\infty N_{\alpha\nu}\,, \quad \alpha = \eta, s\,. \tag{112}$$

Each of such $\eta\nu$ and $s\nu$ configurations involves 2ν anti-bound η-spinons and 2ν bound spinons, respectively. Here $\nu = 1, ...,$ gives the corresponding number of η-spin-singlet anti-bound-η-spinon pairs and spin-singlet bound-spinon pairs, respectively. For $\nu > 1$ the attraction between the ν pairs of each configuration is associated with the imaginary part of the BA rapidity given in Eq. (111). Whether the BA quantum numbers I_j^c of Eq. (99) are integer numbers or half-odd integer numbers is fully determined by the values of the numbers B_η and B_s defined here. The BA quantum

numbers I_j^β in that equation where $\beta = c, \alpha\nu$, $\alpha = \eta, s$, and $\nu = 1, ..., \infty$ are determined by the following boundary conditions,

$$
\begin{aligned}
I_j^\beta &= 0, \pm 1, \pm 2, ... \ \text{ for } G_\beta \text{ even}, \\
&= \pm 1/2, \pm 3/2, \pm 5/2, ... \ \text{ for } G_\beta \text{ odd},
\end{aligned}
\tag{113}
$$

where

$$
G_\beta = \delta_{\beta,c} \sum_{\alpha = \eta, s} B_\alpha + \delta_{\beta, \alpha\nu} [N_c + N_{\alpha\nu} - 1],
\tag{114}
$$

and B_α is defined in Eq. (112). Such values are equivalent to those provided in the text below Eq. (99). From manipulations of the expression provided in Eq. (102), one straightforwardly confirms that $N_{a_{\alpha\nu}} = [N_{\alpha\nu} + N_{\alpha\nu}^h]$ is an odd and even integer number provided that $[N_c + N_{\alpha\nu}]$ is as well an odd and even integer number, respectively.)

Consistent with both the relation between the c fermion and rotated-electron occupancy configurations and the 2ν-spinon ($\alpha = s$) or 2ν-η-spinon ($\alpha = \eta$) composite character of the above $\alpha\nu$ objects, the following exact sum-rules involving summations over the BA quantum numbers q_j in Eqs. (107)-(109) hold,

$$
\begin{aligned}
\sum_{j=1}^{N_a} N_c(q_j) &= N_c = 2S_c, \\
\sum_{j=1}^{N_a} [1 - N_c(q_j)] &= N_c^h = [N_a - 2S_c], \\
\sum_{\nu=1}^{\infty} \sum_{j=1}^{N_{a_{\eta\nu}}} 2\nu \, N_{\eta\nu}(q_j) &= M_\eta^{bo} = [N_a - 2S_c - 2S_\eta], \\
\sum_{\nu=1}^{\infty} \sum_{j=1}^{N_{a_{s\nu}}} 2\nu \, N_{s\nu}(q_j) &= M_s^{bo} = [2S_c - 2S_\eta].
\end{aligned}
\tag{115}
$$

From the use of Eq. (102), one finds that the number $N_{\alpha\nu}^h$ provided in that equation simplifies for $\nu = 1$. It can be expressed only in terms of the number M_α of η-spinons ($\alpha = \eta$) or spinons ($\alpha = s$) and the corresponding configuration number B_α given in Eq. (112) as follows,

$$
N_{\alpha 1}^h = [M_\alpha - 2B_\alpha]; \quad \alpha = \eta, s.
\tag{116}
$$

It is confirmed below that the length $n = \nu = 1, ..., \infty$ of the BA string Λ'^n (and Λ^n) excitations is indeed the number of η-spinon pairs (and spinon pairs) in each of the independent η-spin-singlet (and spin-singlet) configurations. To start with, we call $\eta\nu$ (and $s\nu$) composite particle each of such 2ν-η-spinon (and 2ν-spinon) configurations. For each $\alpha\nu$ momentum band there is one branch of $\alpha\nu$ composite particles. The indices $\alpha = \eta, s$ and $\nu = 1, ..., \infty$ label the distinct branch types of such $\alpha\nu$ composite particles.

Within the $N_a \to \infty$ limit that the thermodynamic BA equations (107)-(109) refer to, it is often convenient to replace the discrete momentum values q_j of Eq. (99), such that $q_{j+1} - q_j = 2\pi/N_a$, by corresponding continuous momentum variables q. Those belong to domains $q \in [-q_\beta, +q_\beta]$ where $\beta = c, \alpha\nu$ whose limiting absolute values q_β read,

$$
\begin{aligned}
q_c &= \pi, \\
q_{\alpha\nu} &= \frac{\pi}{N_a}(N_{a_{\alpha\nu}} - 1) \ \text{ for } N_{a_{\alpha\nu}} \text{ odd}, \\
&= \frac{\pi}{N_a} N_{a_{\alpha\nu}} \ \text{ for } N_{a_{\alpha\nu}} \text{ even}.
\end{aligned}
\tag{117}
$$

For the $\beta = \alpha\nu$ branches the β discrete-momentum values distribution is symmetrical. The $q_{\alpha\nu}$ expression provided in this equation has no $1/N_a$ corrections. Accounting for such c band corrections leads to $q \in [q_c^-, q_c^+]$ where the limiting momentum values $q_c^\pm$ are provided in Eqs. (B.15)-(B.17) of Ref. [21].

The thermodynamic BA equations, Eqs. (107)-(109), refer only to Bethe states. They can be extended to non-LWSs of form given in Eq. (13). This is fulfilled by formally setting some of the rapidities $\Lambda_{\eta\nu}$ and $\Lambda_{s\nu}$ in such equations equal to infinity [39, 40]. For example, Eqs. (3.23b) and (3.24b) of Ref. [39] describe a η-spin non-LWS state with

numbers $S_\eta = 1$ and $S_\eta^{x_3} = 0$. Within our notation, that state rapidity value, $\Lambda_{\eta 1} = \infty$, refers to a η-spin-triplet pair of unbound η-spinons of opposite η-spin projection, rather than to one η-spin-singlet two-spinon composite $\eta 1$ particle. On the other hand, Eqs. (3.23a) and (3.24a) of Ref. [39] describe a Bethe state with numbers $S_\eta = S_\eta^{x_3} = 0$. Its rapidity $\Lambda_{\eta 1}(0)$ refers to such a η-spin-singlet two-η-spinon composite $\eta 1$ particle.

Alternatively, within the present operator formulation the non-LWSs are generated from the corresponding Bethe states by application onto those of the off-diagonal generators of the η-spin or spin $SU(2)$ symmetry algebras, as given in Eq. (13).

B. Consistency of the representations of the model global symmetry algebra with the BA solution and our formulation objects

Here we confirm that the composite $\eta\nu$ particles and composite $s\nu$ particles are η-spin-neutral and spin-neutral objects made out of 2ν η-spinons and 2ν spinons, respectively, where $\nu = 1,...,\infty$. That such 2ν η-spinons and 2ν spinons are in anti-bound and bound configuration states, respectively, is confirmed in Section V G.

1. Three important subspaces

The quantum-number occupancy configurations in the thermodynamic BA equations, Eqs. (107)-(109), generate a well-defined set of Bethe states. Those span the subspace with given fixed values of S_η, S_s, and the sets of numbers $N_c = 2S_c$ and $\{N_{\alpha\nu}\}$ where $\alpha = \eta, s$ and $\nu = 1,...,\infty$. We call it *Takahashi subspace*. The *extended Takahashi subspaces* are spanned by all energy eigenstates with given fixed values of S_η, S_s, and the sets of numbers $N_c = 2S_c$ and $\{N_{\alpha\nu}\}$ where $\alpha = \eta, s$ and $\nu = 1,...,\infty$. That includes as well the non-LWSs states generated from the Bethe states that span the Takahashi subspaces. The dimension of an extended Takahashi subspace then reads,

$$d_{ets} = d_c \times \prod_{\alpha=\eta,s} (2S_\alpha + 1)\, d_{\alpha\nu}\,. \tag{118}$$

The dimensions d_c and $d_{\alpha\nu}$ appearing here are given in Eq. (103) and the S_η and S_s values are fixed. Those read,

$$S_\alpha = \frac{1}{2}\left[M_\alpha - \sum_{\nu=1}^{\infty} 2\nu\, N_{\alpha\nu}\right]\,, \quad \alpha = \eta, s\,, \quad 2S_c \text{ fixed}\,. \tag{119}$$

We divide the Hilbert space of the 1D Hubbard model, Eq. (1), in a set of larger subspaces that contain the extended Takahashi subspaces. They are spanned by the states with fixed values of the numbers $2S_c$, S_η, and S_s. Since the number values of unbound η-spinons, $M_\eta^{un} = 2S_\eta$, and unbound spinons, $M_s^{un} = 2S_s$, are fixed, we call such subspaces *unbound η-spinon and unbound spinon subspaces*. Their dimension is determined by the number $\mathcal{N}(S_s, M_s)$ of M_s-spinon spin $SU(2)$ symmetry algebra state representations, $\mathcal{N}(S_\eta, M_\eta)$ of M_η-η-spinon η-spin $SU(2)$ symmetry algebra state representations, and d_c of $2S_c$-c-fermion c hidden $U(1)$ symmetry algebra state representations at fixed values of the η-spin S_η and spin S_s. (We recall that $M_s = 2S_c$ and $M_\eta = 2S_c^h = [N_a - 2S_c]$.) It reads,

$$d_{u\eta s} = d_c \times \mathcal{N}(S_\eta, M_\eta) \times \mathcal{N}(S_s, M_s)\,. \tag{120}$$

Here the dimension d_c is that provided in Eq. (103) and the two $\alpha = \eta, s$ dimensions $\mathcal{N}(S_\alpha, M_\alpha)$ are given by,

$$\mathcal{N}(S_\alpha, M_\alpha) = (2S_\alpha + 1)\left\{C_{M_\alpha}^{M_\alpha/2 - S_\alpha} - C_{M_\alpha}^{M_\alpha/2 - S_\alpha - 1}\right\}\,, \quad \alpha = \eta, s\,. \tag{121}$$

The sets of numbers $\{N_{\alpha\nu}\}$ where $\alpha = \eta, s$ and $\nu = 1,...,\infty$ of the states that span the smaller extended Takahashi subspaces contained in each of the unbound η-spinon and unbound spinon subspaces have fixed values, which obey the following two sum rules,

$$M_\alpha^{bo} = [M_\alpha - M_\alpha^{un}] = [M_\alpha - 2S_\alpha] = 2\sum_{\nu=1}^{\infty} \nu\, N_{\alpha\nu}\,; \quad \alpha = \eta, s\,. \tag{122}$$

On the other hand, the unbound η-spinon and unbound spinon subspaces considered here are contained in the larger η-spinon and spinon subspaces introduced in Section IV D. Those are spanned by the energy eigenstates with

fixed value for the c fermion number $N_c = 2S_c$, spinon number $M_s = 2S_c$, and η-spinon number $M_\eta = [N_a - 2S_c]$. The dimension of the η-spinon and spinon subspaces is given by,

$$d_{\eta ss} = d_{\eta ss}(2S_c) = \sum_{2S_\eta=0}^{[N_a-2S_c]} \sum_{2S_s=0}^{2S_c} d_c \times \prod_{\alpha=\eta,s} \frac{[1 + (-1)^{[2S_\alpha + 2S_c]}]}{2} \mathcal{N}(S_\alpha, M_\alpha) . \tag{123}$$

The $\sum_{2S_\eta}$ and $\sum_{2S_s}$ summations in this equation run over all consecutive integer numbers $2S_\eta = 0, 1, ..., [N_a - 2S_c]$ and $2S_s = 0, 1, ..., 2S_c$, respectively. The role of the phase factor $(-1)^{[2S_\alpha + 2S_c]}$ is to select only the representations of the model global symmetry algebra, for which both $[2S_\eta + 2S_c]$ and $[2S_s + 2S_c]$ are integer numbers.

Finally, alike in Ref. [19] for general bipartite lattices, summation over the dimensions of all η-spinon and spinon subspaces gives indeed the correct dimension of the 1D Hubbard model Hilbert space,

$$d_{Hil} = \sum_{2S_c=0}^{N_a} d_{\eta ss}(2S_c) = 4^{N_a} . \tag{124}$$

Here the $\sum_{2S_c}$ summation runs over all consecutive integer numbers $2S_c = 0, 1, ..., N_a$.

A side technical question clarified in the introductory discussions of Section I, is how did the authors of Ref. [20] reach the correct number, 4^{N_a}, of energy eigenstates in spite of assuming that the model global symmetry was $SO(4) = [SU(2) \otimes SU(2)]/Z_2^2$ rather than $SO(3) \otimes SO(3) \otimes U(1) = [SO4] \otimes U(1)]/Z_2$? As mentioned in Section I, the answer is simple. To generate the energy eigenstates outside the BA solution, they used the off-diagonal generators of the two non-Abelian $SU(2)$ symmetries. On the other hand, to enumerate the corresponding LWSs $|\Psi_{l_o, l_\triangle^0, u}\rangle$ they used the BA solution, rather than symmetry. Since that solution accounts for the extra c hidden $U(1)$ symmetry algebra representations, they reached the correct number, 4^{N_a}, of energy eigenstates.

2. Confirmation of the $\alpha\nu$ particle composition

The dimension d_c given in Eq. (103) equals the number of occupancy configurations of the $N_c = 2S_c$ c fermions in their c band with N_a discrete momentum values. Their allowed occupancies are 1 and 0. On the other hand, the $\alpha\nu$ composite particles that emerge from the BA solution also carry discrete momentum values q_j whose allowed occupancies are 1 and 0. Thus the number of occupancy configurations of the set of $N_{\alpha\nu}$ $\alpha\nu$ composite particles in their $\alpha\nu$ band with $N_{a_{\alpha\nu}}$ discrete momentum values is that given in Eq. (103), $d_{\alpha\nu} = C_{N_{a_{\alpha\nu}}}^{N_{\alpha\nu}}$. It trivially follows from the η-spin (and spin) $SU(2)$ symmetry algebra that its $\mathcal{N}(S_\eta, M_\eta)$ (and $\mathcal{N}(S_s, M_s)$) representations involve a number of η-spin-singlet (and spin-singlet) representations given by,

$$\mathcal{N}_{singlet}(S_\alpha, M_\alpha) = \frac{\mathcal{N}(S_\alpha, M_\alpha)}{(2S_\alpha + 1)} = C_{M_\alpha}^{M_\alpha/2 - S_\alpha} - C_{M_\alpha}^{M_\alpha/2 - S_\alpha - 1} , \quad \alpha = \eta, s . \tag{125}$$

If the $\eta\nu$ composite particles (and $s\nu$ composite particles) are η-spin neutral (and spin neutral) composite objects of 2ν η-spinons (and 2ν spinons) and, as given in Eq. (122), all corresponding M_α^{bo} η-spinons ($\alpha = \eta$) and spinons ($\alpha = s$) are part of them, the values of their numbers $N_{a_{\alpha\nu}}$ must exactly obey the following equality *for all* unbound η-spinon and unbound spinon subspaces,

$$\sum_{\{N_{\alpha\nu}\}} \prod_{\nu=1}^{\infty} d_{\alpha\nu} = \sum_{\{N_{\alpha\nu}\}} \prod_{\nu=1}^{\infty} C_{N_{a_{\alpha\nu}}}^{N_{\alpha\nu}} = \sum_{\{N_{\alpha\nu}\}} \prod_{\nu=1}^{\infty} C_{N_{a_{\alpha\nu}}}^{N_{\alpha\nu}^h} = \mathcal{N}_{singlet}(S_\alpha, M_\alpha) , \quad \alpha = \eta, s . \tag{126}$$

Here the $\{N_{\alpha\nu}\}$ summation runs over *the whole* set $\nu = 1, ..., \infty$ of $N_{\alpha\nu}$ numbers that owing to the conservation of the $\alpha = \eta, s$ numbers M_η^{bo} and M_s^{bo} exactly obey the subspace sum rules given in Eq. (122). Hence such a summation is over all smaller extended Takahashi subspaces contained in the larger unbound η-spinon and unbound spinon subspaces. The number $\mathcal{N}_{singlet}(S_\alpha, M_\alpha)$ is that given in Eq. (125).

The general dependence of the number $N_{\alpha\nu}^h$ of unoccupied $\alpha\nu$ band discrete momentum values on the S_α value and on those of the set of numbers $\{N_{\alpha\nu'}\}$ where $\nu' = 1, ..., \infty$ is defined by imposing that Eq. (126) is simultaneously obeyed in *all* subspaces. The unique mathematical solution of the problem is indeed that provided by the thermodynamic BA solution of Ref. [1]: Equation (126) is simultaneously obeyed in *all* subspaces provided that the number $N_{a_{\alpha\nu}} = [N_{\alpha\nu} + N_{\alpha\nu}^h]$ of $\alpha\nu$ band discrete momentum values and the corresponding number $N_{\alpha\nu}^h$ of discrete momentum values unoccupied by $\alpha\nu$ composite particles are those provided in Eqs. (101) and (102), respectively. This confirms that the BA solution explicitly accounts for the model global symmetry algebra and corresponding representations.

Moreover, the equality of Eq. (126) confirms that the $\eta\nu$ band (and $s\nu$ band) occupancy configurations refer to η-spin-neutral (and spin-neutral) η-spinon (and spinon) occupancy configurations. Hence they generate representations of the $U(1)$ symmetry sub-algebra within the η-spin (and spin) $SU(2)$ symmetry algebra. On the other hand, the unbound η-spinon (and unbound spinon) occupancies generate the remaining representations the η-spin (and spin) $SU(2)$ symmetry algebra.

Within chromodynamics, the quarks have color but all quark-composite physical particles are color-neutral [51]. Here the M_η^{bo} η-spinons (and M_s^{bo} spinons) that are not invariant under the electron - rotated-electron unitary transformation have η-spin $1/2$ (and spin $1/2$) but the corresponding 2ν-η-spinon $\eta\nu$ composite particles (and 2ν-spinon $s\nu$ composite particles) are η-spin neutral (and spin neutral).

C. Subspace dependent $\alpha\nu$ composite particles statistics

A quantum problem is defined by a Hamiltonian and the subspace it acts onto. Hence the 1D Hubbard model in each of the three subspaces considered above in Section V B corresponds to three distinct quantum problems. Here we show that for each of such three quantum problems the $\alpha\nu$ composite particles have a different statistics, as classified according to the generalized principle of Ref. [31].

In all the three subspaces the number of c fermions is fixed and given by the eigenvalue of the c hidden $U(1)$ symmetry generator, $N_c = 2S_c$. Since the η-spinon and spinon operator algebra refers to the η-spinon and spinon subspace, the dimension relevant for deriving the statistical interaction $g_{\alpha\nu,\alpha'\nu'} = \delta_{\alpha,\alpha'} \, g_{\nu,\nu'}$ reads,

$$\mathcal{N}_{\alpha\nu} = 1 + N_{\alpha\nu}^h \, . \tag{127}$$

The statistical interaction is related to the changes $\delta\mathcal{N}_{\alpha\nu}$ of the dimension given here as a result of the deviations $\delta N_{\alpha\nu'}$ in the $\alpha\nu'$ composite particle numbers where $\nu' = 1, ..., \infty$. The statistical interaction does not connect $\eta\nu$ and $s\nu'$ branches, consistently with those being associated with independent η-spin and spin degrees of freedom, respectively.

The statistical interaction $g_{\alpha\nu,\alpha'\nu'} = \delta_{\alpha,\alpha'} \, g_{\nu,\nu'}$ is defined by the equation,

$$\delta\mathcal{N}_{\alpha\nu} = - \sum_{\nu'=1}^{\infty} g_{\nu,\nu'} \, \delta N_{\alpha\nu'} \, . \tag{128}$$

1. The $\alpha\nu$ composite particles statistics in the η-spinon and spinon subspaces

In the η-spinon and spinon subspaces the c fermion number $N_c = 2S_c$, spinon number $M_s = 2S_c$, and η-spinon number $M_\eta = [N_a - 2S_c]$ have fixed values. The conservation of M_α for $\alpha = \eta, s$ implies that the set of deviations δM_α^{un} and $\{\delta N_{\alpha\nu}\}$ where $\nu = 1, ..., \infty$ must obey the sum rule,

$$\delta M_\alpha = \delta M_\alpha^{un} + \sum_{\nu=1}^{\infty} 2\nu \, \delta N_{\alpha\nu} = 0 \, , \quad \alpha = \eta, s \, . \tag{129}$$

In order to classify the statistics of the $\alpha\nu$ composite particles according to the generalized principle of Ref. [31], it is convenient to rewrite the number of $\alpha\nu$ band holes given in Eq. (102) as follows,

$$N_{\alpha\nu}^h = [M_\alpha - \sum_{\nu'=1}^{\infty} (\nu + \nu' - |\nu - \nu'|) N_{\alpha\nu'}] \, , \quad M_\alpha \text{ fixed} \, , \quad \alpha = \eta, s \, . \tag{130}$$

From the use of Eqs. (127)-(130) one readily finds the following $\alpha\nu$ composite particle statistical interaction $g_{\nu,\nu'}$ for the quantum problem defined by the 1D Hubbard model in the η-spinon and spinon subspace,

$$g_{\nu,\nu'} = (\nu + \nu' - |\nu - \nu'|) \, , \quad \nu, \nu' = 1, ..., \infty \, . \tag{131}$$

Hence for that quantum problem the $\alpha\nu$ composite particles are neither fermions ($g_{\nu,\nu'} = \delta_{\nu,\nu'}$) nor bosons ($g_{\nu,\nu'} = 0$).

2. The $\alpha\nu$ composite particles statistics in the unbound η-spinon and unbound spinon subspaces

In the unbound η-spinon and unbound spinon subspaces the η-spin S_η and spin S_s values are fixed, along with those of the c fermion number $N_c = 2S_c$, spinon number $M_s = 2S_c$, and η-spinon number $M_\eta = [N_a - 2S_c]$. The conservation of such numbers implies that the set of deviations $\{\delta N_{\alpha\nu}\}$ where $\nu = 1, ..., \infty$ must obey the sum rule,

$$\sum_{\nu=1}^{\infty} \nu \, \delta N_{\alpha\nu} = 0 \,. \tag{132}$$

In order to classify the statistics of the $\alpha\nu$ composite particles according to the generalized principle, the suitable expression for the number of $\alpha\nu$ band holes is that given in Eq. (102). By combining such an expression with Eqs. (127) and (128) we readily find the following $\alpha\nu$ composite particle statistical interaction $g_{\nu,\nu'}$ for the quantum problem defined by the 1D Hubbard model in the unbound η-spinon and unbound spinon subspace,

$$\begin{aligned} g_{\nu,\nu'} &= 0 \,, \quad \nu = 1, ..., \infty \,, \quad \nu' \leq \nu \,, \\ &= -2(\nu' - \nu) \,, \quad \nu = 1, ..., \infty \,, \quad \nu' > \nu \,. \end{aligned} \tag{133}$$

Again for that quantum problem the $\alpha\nu$ composite particles are neither fermions nor bosons.

3. The $\alpha\nu$ composite particles statistics in the $\delta N_{\alpha\nu}^h = 0$ subspaces and extended Takahashi subspaces

A $\delta N_{\alpha\nu}^h = 0$ subspace is a subspace of a unbound η-spinon and unbound spinon subspace for which the number $N_{\alpha\nu}^h$ vanishes for a specific $\alpha\nu$ branch and $\delta N_{\alpha\nu'} = 0$ for all $\nu' > \nu$ branches. The conservation of $N_{\alpha\nu}^h$ and $\{N_{\alpha\nu}\}$ for $\nu' > \nu$, along with that of the unbound η-spinon and unbound spinon subspace numbers, implies that the set of deviations $\{\delta N_{\alpha\nu'}\}$ where $\nu' = 1, ..., \nu$ must obey the sum rule,

$$\sum_{\nu'=1}^{\nu} \nu' \, \delta N_{\alpha\nu'} = 0 \,. \tag{134}$$

Therefore, for the quantum problem defined by the 1D Hubbard model in such a subspace the $\alpha\nu$ composite particle statistical interaction $g_{\nu,\nu'}$ is a particular case of that provided in Eq. (133) given by,

$$g_{\nu,\nu'} = 0 \,. \tag{135}$$

It then follows that for such quantum problem the $\alpha\nu$ composite particles are bosons.

That the concerning the site occupancy configurations of the $\alpha\nu$ effective lattice the $\alpha\nu$ composite particles behave actually as hard-core bosons and thus the corresponding $\alpha\nu$ operators generated from theirs by a Jordan-Wigner transformation obey an anticommuting algebra is consistent with the following properties:

– An anticommuting algebra for both the c fermion operators of Eq. (105) and the $\alpha\nu$ operators obtained from those of the hard-core bosonic $\alpha\nu$ composite particles generates from the electron and rotated-electron vacuum a faithful representation of the energy eigenstates that span the $\delta N_{\alpha\nu}^h = 0$ subspaces and extended Takahashi subspaces. This applies to all the model 4^{N_a} energy eigenstates, since each of them belongs to a $\delta N_{\alpha\nu}^h = 0$ subspace and extended Takahashi subspace associated with a well-defined initial ground state.

– Such an energy eigenstate representation involves the $\alpha\nu$ band discrete momentum values $q_j = I_j^{\alpha\nu} [2\pi/N_a]$ of Eq. (99) in the momentum general expression given in Eq. (104) provided that they are carried by $\alpha\nu$ objects whose anticommuting operators are generated from those of $\alpha\nu$ composite particles. This is consistent with within the exact BA solution the set of $\alpha\nu$ quantum numbers $I_j^{\alpha\nu}$ of Eq. (113) for $\beta = \alpha\nu$ and $j = 1, ..., N_{a_{\alpha\nu}}$ with $N_{a_{\alpha\nu}}$ defined by Eqs. (101) and (102), which are the above discrete momentum values $q_j = I_j^{\alpha\nu} [2\pi/N_a]$ in units of $[2\pi/N_a]$, having for all energy eigenstates Pauli-like allowed occupancies 0 and 1, respectively. This is alike the occupancies 0 and 1 of the BA c quantum numbers I_j^c associated with the $\beta = c$ band discrete momentum values $q_j = I_j^c [2\pi/N_a]$, which are carried by the c fermions whose operators are given in Eq. (105) and obey the anticommuting algebra of Eq. (106).

– The discrete momenta $q_j = [2\pi/N_a] I_j^\beta$ provided in Eq. (99) with the quantum numbers I_j^β values as given in Eq. (113) by the exact BA solution are also exactly those that emerge from the boundary conditions brought about by the Jordan-Wigner transformation that generates $\alpha\nu$ *fermions* from the hard-core bosonic $\alpha\nu$ composite particles.

– The dynamical and spectral function expressions derived for general u values within the PDT of Refs. [8–11] agree in the $u \gg 1$ limit with those of the method of Ref. [52] provided that alike the c fermion operators of Eqs. (105) and (106), the $s1$ operators obtained from those of the $s1$ composite particles obey anticommutation relations. Within the scattering theory introduced in the second paper, the c and $s1$ pseudofermion operators generated from the anticommuting c and $s1$ fermion operators, respectively, have modified phase-shift dependent exotic anticommutators that control the PDT quantum overlaps of the dynamical and spectral function matrix elements between the ground state and the excited states. (Within the method of Ref. [52], which is valid for $u \gg 1$, the charge degrees of freedom are described by spinless fermions that refer to the c fermions, whereas the spin degrees of freedom are described by the wave function of the 1D spin-1/2 isotropic Heisenberg model.)

Hence we rename the the $\alpha\nu$ composite particles, $\alpha\nu$ *bond particles*. The $\alpha\nu$ effective lattices are defined below. Their introduction simplifies the description of some particular types of the spin ($\alpha = s$) or η-spin ($\alpha = \eta$) effective lattice occupancy configurations.

For the particular case of the $\alpha1$ branches, Eq. (134) is only fulfilled for an extended Takahashi subspace. An extended Takahashi subspace is a $\delta N_{\alpha\nu}^h = 0$ subspaces for *all* its $\alpha\nu$ bands with finite occupancy. For it the same numbers as for a unbound η-spinon and unbound spinon subspace are fixed, along with those of the sets of $\alpha\nu$ composite bound-particle numbers $\{N_{\alpha\nu}\}$ where $\alpha = \eta, s$ and $\nu = 1, ..., \infty$. The Bethe states contained in such subspaces span the Takahashi subspaces associated with the thermodynamic BA equations, Eqs. (107)-(109). It then follows from Eq. (102) that numbers of $\alpha\nu$ band holes are fixed as well. In general we consider that the the the $\delta N_{\alpha\nu}^h = 0$ subspaces are extended Takahashi subspaces.

D. The $\alpha\nu$ fermions emerging from the hard-core $\alpha\nu$ bond particles

Above we have established that the spinons (and η-spinons) that are not invariant under the electron rotated-electron transformation are part of spin (and η-spin) neutral 2ν-spinon (and 2ν-η-spinon) composite $s\nu$ (and $\eta\nu$) bond particles.

The concept of a $\alpha\nu$ effective lattice is well-defined in the extended Takahashi subspaces. For the 1D Hubbard model in such subspaces, the numbers $N_{a_{\alpha\nu}}$, $N_{\alpha\nu}$, and $N_{\alpha\nu}^h$ in Eqs. (101) and (102) give as well the numbers of the $\alpha\nu$ effective lattice sites, occupied sites, and unoccupied sites, respectively. An occupied site of the $\alpha\nu$ effective lattice corresponds to $2\nu = 2, 4, ..., \infty$ sites of the η-spin ($\alpha = \eta$) or spin ($\alpha = s$) effective lattice. Consistent with the expressions provided in Eqs. (101) and (102), the $2S_\eta$ (and $2S_s$) sites of the η-spin (and spin) effective lattice occupied by unbound η-spinons (and unbound spinons) and $2(\nu' - \nu)$ sites out of the $2\nu'$ sites of that lattice occupied by each hard-core $\eta\nu'$ (and $s\nu'$) bond particle such that $\nu' > \nu$ play the role of unoccupied sites of the $\eta\nu$ (and $s\nu$) effective lattice.

Provided that the ratio $N_{a_{\alpha\nu}}/N_a$ remains finite as $N_a \to \infty$, the $\alpha\nu$ effective lattices can be represented by 1D lattices with spacing,

$$a_{\alpha\nu} = \frac{L}{N_{a_{\alpha\nu}}} = \frac{N_a}{N_{a_{\alpha\nu}}} a = \frac{N_{a_\beta}}{N_{a_{\alpha\nu}}} a_\alpha ; \quad N_{a_{\alpha\nu}} \geq 1 , \tag{136}$$

where $\nu = 1, ..., \infty$ and $\alpha = \eta, s$. The arguments behind the 1D $\alpha\nu$ effective lattice average distance $a_{\alpha\nu}$ between its sites playing the role of lattice spacing are similar to those used in Section IV A for the spacing of the η-spin and spin effective lattices.

The traditional operational formalism of second quantization can be applied to the $\alpha\nu$ bond particles for transitions within the extended Takahashi subspaces. Indeed, for such subspaces the dimension $\mathcal{N}_{\alpha\nu} = [1 + N_{\alpha\nu}^h]$ of Eq. (127) remains constant. In terms of the occupancies of the $\alpha\nu$ band discrete momentum values, such transitions involve particle-hole processes. As discussed below, the $\alpha\nu$ bond particle creation or annihilation operators also play a role in transitions between different extended Takahashi subspaces whose description is beyond the standard operational formalism of second quantization.

Hence one may introduce creation and annihilation operators for the $\alpha\nu$ bond particles provided that they are used in the expressions of the generators of the allowed processes and transitions. In addition, such operators must obey an algebra compatible with the $\alpha\nu$ bond particles being hard-core bosons. Thus the operators $g_{j,\alpha\nu}^\dagger$ and $g_{j,\alpha\nu}$ that create and annihilate one $\alpha\nu$ bond particle at a $\alpha\nu$ effective lattice site of index $j = 1, ..., N_{a_{\alpha\nu}}$ must anticommute on the same site,

$$\{g_{j,\alpha\nu}^\dagger, g_{j,\alpha\nu}\} = 1 ; \quad \{g_{j,\alpha\nu}^\dagger, g_{j,\alpha\nu}^\dagger\} = \{g_{j,\alpha\nu}, g_{j,\alpha\nu}\} = 0 , \tag{137}$$

and commute on different sites,

$$[g_{j,\alpha\nu}^\dagger, g_{j',\alpha\nu}] = [g_{j,\alpha\nu}^\dagger, g_{j',\alpha\nu}^\dagger] = [g_{j,\alpha\nu}, g_{j',\alpha\nu}] = 0 ; \quad j \neq j' . \tag{138}$$

Such $\eta\nu$ (and $s\nu$) bond-particle operators can be expressed in terms of products of η-spinon (and spinon) operators, Eq. (67). Since their expressions involve only such operators, it follows from Eq. (77) that they commute with the c fermion operators,

$$[f_{j,c}^\dagger, g_{j',\alpha\nu}^\dagger] = [f_{j,c}, g_{j',\alpha\nu}^\dagger] = [f_{j,c}^\dagger, g_{j',\alpha\nu}] = [f_{j,c}, g_{j',\alpha\nu}] = 0\,, \quad \alpha = \eta, s\,, \quad \nu = 1, ..., \infty\,. \tag{139}$$

Each site of the $\eta\nu$ (and $s\nu$) effective lattice refers to 2ν sites of the η-spin (and spin) effective lattice. For each occupancy configurations of the latter effective lattice, the 2ν sites of a $\eta\nu$ (and $s\nu$) bond particle are neither occupied by another $\eta\nu'$ (and $s\nu'$) bond particle of a different $\nu' \neq \nu$ branch nor by unbound η-spinons (and unbound spinons). Moreover, the sites of the η-spin and spin effective lattice correspond to different sites of the original lattice. Hence it follows from the η-spinon and spinon operator algebra of Eq. (79) that the operators of $\alpha\nu$ and $\alpha'\nu'$ bond particles corresponding to different $\alpha\nu \neq \alpha'\nu'$ branches commute between themselves,

$$[g_{j,\alpha\nu}^\dagger, g_{j',\alpha'\nu'}] = [g_{j,\alpha\nu}^\dagger, g_{j',\alpha'\nu'}^\dagger] = [g_{j,\alpha\nu}, g_{j',\alpha'\nu'}] = 0\,; \quad \alpha\nu \neq \alpha'\nu'\,. \tag{140}$$

When acting onto their extended Takahashi subspace, the $\alpha\nu$ bond-particle creation and annihilation operators appear in operators whose expressions contain an equal number of such creation and annihilation operators. However, they also appear in expressions of operators containing only $\alpha\nu$ bond particle creation or annihilation operators. Specifically, this is the case of the operators that generate transitions between extended Takahashi subspaces belonging to the same η-spinon and spinon subspace. Those can be written as a product of two operators. One of them adds or removes lattice sites to or from, respectively, the initial subspace $\alpha\nu$ effective lattices. The other operator is one or a product of $\alpha\nu$ bond-particle creation or annihilation operators suitable to the final subspace. We note that adding or removing $\alpha\nu$ effective lattice sites also adds and removes, respectively, discrete momentum values from the corresponding $\alpha\nu$ momentum band.

Analysis of the spectral-weight distributions obtained by use of the PDT formalism [8–11] reveals that most $\eta\nu$ (and $s\nu$) bond particle spectral weight corresponds to a 2ν-site compact domain of the former lattice. The spatial coordinate $x_j = a_{\eta\nu}\, j$ (and $x_j = a_{s\nu}\, j$) of the $\eta\nu$ (and $s\nu$) bond particle refers to the position of such a domain middle point. However, more diluted and thus spread 2ν-site η-spin (and spin) effective lattice occupancy configurations of increasing length but centered at that point contribute as well to the $\eta\nu$ (and $s\nu$) bond particle.

Fortunately, within the $N_a \gg 1$ limit associated with our operator description the problem of the internal degrees of freedom of the composite $\alpha\nu$ bond particles separates from that of their position in the corresponding $\alpha\nu$ effective lattice. The latter corresponds to the spatial coordinate of the above η-spin lattice ($\alpha = \eta$) or spin lattice ($\alpha = s$) middle point of each $\alpha\nu$ bond particle 2ν-sites configuration. Hence here we do not need to address the very complex problem of the explicit expression of the $\eta\nu$ (and $s\nu$) bond particle operators in terms of products of η-spinon (and spinon) operators, which is implicitly accounted for by the BA solution.

Within the Jordan-Wigner transformation method of Ref. [53], the hard-core $\alpha\nu$ bond particles are mapped into $\alpha\nu$ fermions with operators given by,

$$f_{j,\alpha\nu}^\dagger = e^{i\phi_{j,\alpha\nu}}\, g_{j,\alpha\nu}^\dagger\,; \quad f_{j,\alpha\nu} = e^{-i\phi_{j,\alpha\nu}}\, g_{j,\alpha\nu}\,, \tag{141}$$

where,

$$\phi_{j,\alpha\nu} = \sum_{j' \neq j} f_{j',\alpha\nu}^\dagger f_{j',\alpha\nu}\, \phi_{j',j,\alpha\nu}\,. \tag{142}$$

For 1D the phase $\phi_{j',j,\alpha\nu}$ appearing here has for all $\alpha\nu$ branches only two possible values, $\phi_{j',j,\alpha\nu} = 0$ and $\phi_{j',j,\alpha\nu} = \pi$. Indeed, the relative angle between two sites of the $\alpha\nu$ effective lattice in a 1D chain can only be one of the two values. Then the $\alpha\nu$ phase factor of Eq. (142) is such that [53],

$$e^{i(\phi_{j+1,\alpha\nu} - \phi_{j,\alpha\nu})} = e^{i\pi\, f_{j,\alpha\nu}^\dagger f_{j,\alpha\nu}}\,. \tag{143}$$

The c fermion operators have the anticommuting relations given in Eq. (76). On the other hand, the $\alpha\nu$ fermion operators that emerge from the Jordan-Wigner transformation associated with Eqs. (141) and (142) have similar anticommuting relations given by,

$$\{f_{j,\alpha\nu}^\dagger, f_{j',\alpha\nu}\} = \delta_{j,j'}\,; \quad \{f_{j,\alpha\nu}^\dagger, f_{j',\alpha\nu}^\dagger\} = \{f_{j,\alpha\nu}, f_{j',\alpha\nu}\} = 0\,. \tag{144}$$

In addition, it follows from Eqs. (139)-(142) that the $\alpha\nu$ fermion operators commute with those of the c fermions,

$$[f_{j,c}^\dagger, f_{j',\alpha\nu}^\dagger] = [f_{j,c}, f_{j',\alpha\nu}^\dagger] = [f_{j,c}^\dagger, f_{j',\alpha\nu}] = [f_{j,c}, f_{j',\alpha\nu}] = 0\,, \quad \alpha = \eta, s\,, \quad \nu = 1, ..., \infty\,, \tag{145}$$

and $\alpha\nu$ and $\alpha'\nu'$ fermion operators corresponding to different $\alpha\nu \neq \alpha'\nu'$ branches commute between themselves,

$$[f_{j,\alpha\nu}^\dagger, f_{j',\alpha'\nu'}] = [f_{j,\alpha\nu}^\dagger, f_{j',\alpha'\nu'}^\dagger] = [f_{j,\alpha\nu}, f_{j',\alpha'\nu'}] = 0 \; ; \quad \alpha\nu \neq \alpha'\nu' \,. \tag{146}$$

One can introduce $\alpha\nu$ fermion operators $f_{q_j,\alpha\nu}^\dagger$ labeled by discrete momentum values q_j such that $j = 1, ..., N_{a_{\alpha\nu}}$. Those are the conjugate variables of the $\alpha\nu$ effective lattice real-space coordinates of site index $j = 1, ..., N_{a_{\alpha\nu}}$. It is confirmed below that their values exactly coincide with those of the BA solution discrete momentum values given in Eq. (99). For subspaces for which the ratio $N_{a_{\alpha\nu}}/N_a$ involving the number $N_{a_{\alpha\nu}}$ of sites of the $\alpha\nu$ effective lattice given in Eqs. (101) and (102) is finite, such operators are given by,

$$f_{q_j,\alpha\nu}^\dagger = \frac{1}{\sqrt{N_{a_{\alpha\nu}}}} \sum_{j'=1}^{N_{a_{\alpha\nu}}} e^{+iq_j a_{\alpha\nu} j'} f_{j',\alpha\nu}^\dagger \,, \quad j = 1, ..., N_{a_{\alpha\nu}} \,,$$

$$f_{q_j,\alpha\nu} = \frac{1}{\sqrt{N_{a_{\alpha\nu}}}} \sum_{j'=1}^{N_{a_{\alpha\nu}}} e^{-iq_j a_{\alpha\nu} j'} f_{j',\alpha\nu} \,, \quad j = 1, ..., N_{a_{\alpha\nu}} \,. \tag{147}$$

Note that $L = a_{\alpha\nu} N_{a_{\alpha\nu}}$.

In 1D the phase factor $e^{i\phi_{j,\alpha\nu}}$ does not have any effect when operating before $f_{j,\alpha\nu}^\dagger$. It follows that in 1D the expression of the Hamiltonian does not involve the phases $\phi_{j,\alpha\nu}$ given in Eq. (142). On the other hand, the Jordan-Wigner transformation phases $\phi_{j,\alpha\nu}$ have direct effects on the boundary conditions. Those determine the discrete momentum values q_j of both the c and $\alpha\nu$ fermion operators of Eqs. (63) and (147), respectively. In 1D the periodic boundary conditions of the original electron problem are ensured provided that one accounts for the effects of the Jordan-Wigner transformation on the boundary conditions of the c fermions and $\alpha\nu$ fermions upon moving one of such objects around the chain of length L once. That in 1D only the values $\phi_{j',j,\alpha\nu} = 0$ and $\phi_{j',j,\alpha\nu} = \pi$ are allowed in the $\phi_{j,\alpha\nu}$ expression given in Eq. (142) implies that in units of $2\pi/L$ the $\alpha\nu$ fermion discrete momentum values either are integer numbers or half-odd integer numbers.

We recall that the rotated-electron occupancies of the sites of the original lattice separate into two degrees of freedom only. Those of the $N_R^s = 2S_c$ sites of the original lattice singly occupied by rotated electrons separate into (i) $N_c = N_R^s = 2S_c$ sites of the c effective lattice occupied by c fermions and (ii) $N_{a_s} = M_s = N_R^s = 2S_c$ sites of the spin effective lattice occupied by spinons. Those of the $N_R^\eta = [N_a - 2S_c]$ sites of the original lattice doubly occupied and unoccupied by rotated electrons separate into (i) $N_c^h = 2S_c^h = N_R^\eta = [N_a - 2S_c]$ sites of the c effective lattice unoccupied by c fermions and (ii) $N_{a_\eta} = M_\eta = 2S_c^h = N_R^\eta = [N_a - 2S_c]$ sites of the η-spin effective lattice occupied by η-spinons. Indeed, the number values equalities $N_c = M_s = N_R^s$ and $N_c^h = M_\eta = N_R^\eta$ given in Eq. (100) do not imply a similar equality for the objects under consideration. Specifically, the N_c c fermions (and N_c^h c fermion holes) and M_s spin-1/2 spinons (and M_η η-spin-1/2 η-spinons) describe different degrees of freedom of the same N_R^s rotated-electron singly occupied sites (and N_R^η rotated-electron doubly occupied and unoccupied sites) whose rotated-electron site occupancy numbers are defined in Eqs. (10) and (11).

The c fermions do not emerge from a Jordan-Wigner transformation. On the other hand, each $\alpha\nu$ fermion corresponds to a set of 2ν sites of the original lattice different from and independent of those of any other $\alpha'\nu'$ fermion. It then follows that upon moving around its $\alpha\nu$ effective lattice of length L, a $\alpha\nu$ fermion only feels the Jordan-Wigner-transformation phases of its own lattice. Those are associated with both the $\alpha\nu$ fermions and $\alpha\nu$ fermion holes. Hence its discrete momentum values obey the following periodic or anti-periodic boundary conditions,

$$e^{iq_j L} = \prod_{j=1}^{N_{a_{\alpha\nu}}} \left\{ \left[e^{i(\phi_{j+1,\alpha\nu} - \phi_{j,\alpha\nu})} \right]^\dagger e^{i(\phi_{j+1,\alpha\nu} - \phi_{j,\alpha\nu})} \right\} = e^{i\pi[N_{a_{\alpha\nu}} - 1]} = -e^{i\pi N_{a_{\alpha\nu}}} \,. \tag{148}$$

Here the phase factor reads 1 and -1 for $[N_{a_{\alpha\nu}} - 1]$ even and odd, respectively. The term -1 in $[N_{a_{\alpha\nu}} - 1]$ can be understood as referring to the site occupied by the $\alpha\nu$ fermion moving around its effective lattice, which must be excluded.

For the $\alpha\nu$ fermions the unoccupied sites of their $\alpha\nu$ effective lattice exist in their own right. Indeed, note that according to Eq. (141) the expression of both the creation and annihilation operators of such objects involve the Jordan-Wigner-transformation phase $\phi_{j,\alpha\nu}$. As a result, such a phase affects both the $\alpha\nu$ fermions and $\alpha\nu$ fermion holes. That justifies why the phase factor $e^{i\pi[N_{a_{\alpha\nu}} - 1]}$ of Eq. (148) involves all the $N_{a_{\alpha\nu}} = [N_{\alpha\nu} + N_{\alpha\nu}^h]$ sites of the $\alpha\nu$ effective lattice. The only exception is that occupied by the moving $\alpha\nu$ fermion. Hence it involves both the $[N_{\alpha\nu} - 1]$ sites occupied by the remaining fermions of the same $\alpha\nu$ branch and the corresponding $N_{\alpha\nu}^h$ $\alpha\nu$ fermion holes.

In contrast, the c fermions are only affected by the sites occupied by $\alpha\nu$ fermions. Indeed, only the sets of 2ν sites of the spin (and η-spin) effective lattice associated with each occupied site of the $s\nu$ (and $\eta\nu$) $\nu = 1, ..., \infty$ effective
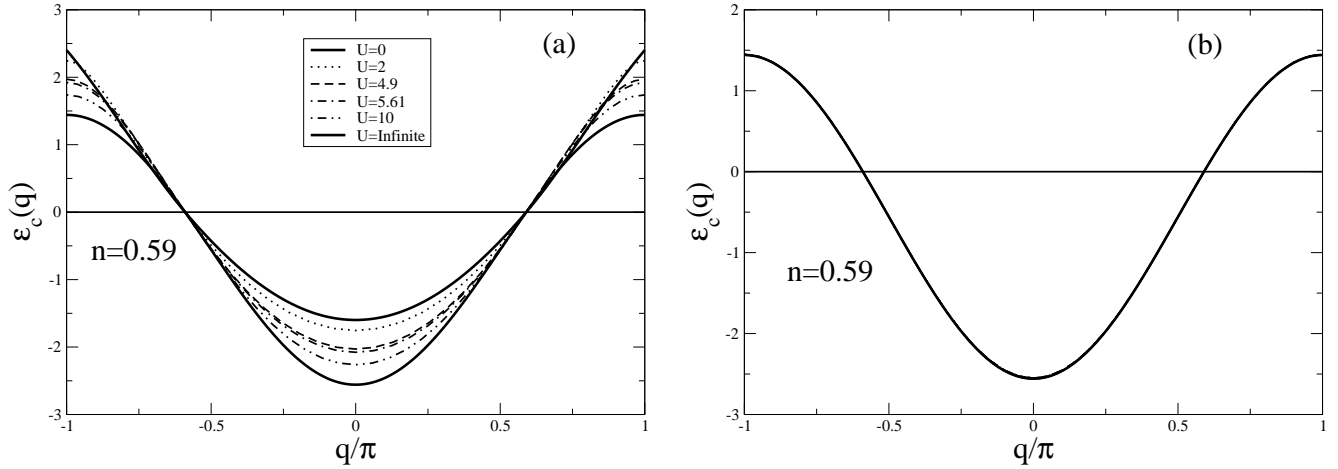
FIG. 1: The c fermion energy dispersion $\varepsilon_c(q) = \varepsilon_c^0(q) - \varepsilon_c^0(q_{Fc})$ defined by Eqs. (161) and (162) for $\beta = c$ plotted as a function of the momentum in units of t for a set of U values (in units of t), electronic density $n = 0.59$, and (a) spin density $m = 0$ and (b) limit of maximum spin density $m \to n = 0.59$. In the spin-density $m \to n$ limit the shape of the energy dispersion $\varepsilon_c(q)$ becomes independent of U/t. In both figures the vanishing-energy ground-state energy level is marked by a horizontal line, which overlaps the energy dispersion at the c Fermi points $q = \pm q_{Fc} = \pm 2k_F = \pm \pi n$.

lattices and the sites of the spin (and η-spin) effective lattice occupied by unbound spinons (and unbound η-spinons) correspond to sites of the original lattice whose degrees of freedom associated with the c hidden $U(1)$ symmetry are described by the occupancy configurations of the c effective lattice.

The unbound spinons and unbound η-spinons of η-spin projection $+1/2$ do not contribute to the states momentum. The momentum π associated with the unbound η-spinons of η-spin projection $-1/2$ remains unchanged for all Hilbert-space energy eigenstates. Consistent, unbound spinons and unbound η-spinons do not undergo any Jordan-Wigner transformation. Thus they do not play any role in the boundary condition that determines the c band momentum values. On the other hand, due to the Jordan-Wigner-transformation phase $\phi_{j',\alpha\nu}$ of each of the $N_{\alpha\nu}$ $\alpha\nu$ fermions at sites $j' = 1, ..., N_{a_{\alpha\nu}}$ of their $\alpha\nu$ effective lattice, the c fermion discrete momentum values are determined by the following periodic or anti-periodic boundary condition,

$$e^{iq_j L} = \prod_{\alpha\nu} \prod_{j'=1}^{N_{\alpha\nu}} e^{i(\phi_{j'+1,\alpha\nu} - \phi_{j',\alpha\nu})} = e^{i\pi \sum_{\alpha\nu} N_{\alpha\nu}}. \tag{149}$$

The phase factor on the right-hand side of Eq. (149) reads 1 and -1 for $\sum_{\alpha\nu} N_{\alpha\nu}$ even and odd, respectively.

The above results imply that the discrete momentum values q_j of both c and $\alpha\nu$ fermions have the usual momentum spacing $q_{j+1} - q_j = 2\pi/L$. Moreover, they are exactly those of the BA solution given in Eq. (99). Here the same values of the quantum numbers $I_j^{\alpha\nu}$ and I_j^c given in Eq. (113) were imposed by the boundary conditions of Eqs. (148) and (149). This is fully consistent with the discrete momentum values of Eq. (99) being within our operator formulation carried by the c fermions and $\alpha\nu$ fermions as defined here.

E. The general energy spectrum, the β fermion energy dispersions, and the Hamiltonian expression

Let us denote the c and $\alpha\nu$ fermions by β fermions, where $\beta = c, \alpha\nu$. The corresponding momentum distributions $N_\beta(q_j)$ appearing in the functional representations of the total momentum provided in Eq. (104) and thermodynamic BA equations given in Eqs. (107)-(109) are the eigenvalues of the number operators,

$$\hat{N}_\beta(q_j) = f_{q_j,\beta}^\dagger f_{q_j,\beta}, \quad \beta = c, \alpha\nu. \tag{150}$$

As mentioned in Section V A, such operators commute with the 1D Hubbard model Hamiltonian. Consistent, the Bethe states are eigenstates of the number operators provided in Eq. (150). Those have eigenvalues $N_\beta(q_j) = 1$ for occupied momentum values and $N_\beta(q_j) = 0$ for unoccupied momentum values. The non-LWSs generated from such Bethe states differ from them only in the unbound η-spinon and unbound spinon occupancies. Hence the c fermion and

$\alpha\nu$ fermion operator algebras and corresponding occupancy configurations apply to all energy eigenstates, including those outside the BA solution subspace.

The quantum numbers in the thermodynamic BA equations, Eqs. (107) and (108), are the discrete momentum values q_j of Eq. (99). Those are eigenvalues of corresponding β translation generators $\hat{q}_\beta$, which commute with the Hamiltonian, momentum operator, and electron - rotated-electron unitary operator. That the rotated-electron occupancy configurations that generate the Bethe states, $|\Psi_{l_o,l_\triangle^0,u}\rangle$, are for $u > 0$ independent of u is consistent with the corresponding β fermion momentum values q_j occupancy configurations being also independent of u. On the other hand, the corresponding rapidity momentum functions $k_c(q_j)$ and rapidity functions $\Lambda_{\alpha\nu}(q_j)$ appearing in the thermodynamic BA equations, Eqs. (107)-(109), are the eigenvalues of corresponding operators,

$$\hat{k}_c(q_j)\,; \quad \hat{\Lambda}_{\alpha\nu}(q_j)\,, \quad \alpha = \eta, s\,, \quad \nu = 1, ..., \infty\,. \tag{151}$$

Such operators also commute with the 1D Hubbard model Hamiltonian. Thus the Bethe states are eigenstates of the rapidity operators. However, except for $u \to \infty$ they do not commute with the electron - rotated-electron unitary operator.

The rapidity operators of Eq. (151) have a well-defined expression in terms of the sets of number operators $\hat{N}_c(q_j)$ and $\{\hat{N}_{\alpha\nu}(q_j)\}$ of Eq. (150) where $\alpha = \eta, s$ and $\nu = 1, ..., \infty$. The dependence of such rapidity operators on the latter number operators has exactly the same form as that of the corresponding BA rapidities $k_c(q_j)$ and $\Lambda_{\alpha\nu}(q_j)$ on the set of momentum distributions $N_c(q_j)$ and $\{N_{\alpha\nu}(q_j)\}$ where again $\alpha = \eta, s$ and $\nu = 1, ..., \infty$. The latter dependence is defined by the thermodynamic BA, Eqs. (107)-(109). Hence such equations define as well the rapidity operators of Eq. (151).

At both finite chemical potential and magnetic field the relation provided in Eq. (B3) of Appendix B between the energy eigenvalues $E = \langle\Psi_{l_o,l_\triangle,u}|\hat{H}|\Psi_{l_o,l_\triangle,u}\rangle$ and $E_{symm} = \langle\Psi_{l_o,l_\triangle,u}|\hat{H}_{symm}|\Psi_{l_o,l_\triangle,u}\rangle$ of the Hamiltonians (1) and (2), respectively, can be rewritten as,

$$E = E_{symm} + \mu\left[M^{un}_{\eta,+1/2} - M^{un}_{\eta,-1/2}\right] + \mu_B H\left[M^{un}_{s,+1/2} - M^{un}_{s,-1/2}\right]. \tag{152}$$

As found in Ref. [1], here the energy eigenvalues E_{symm} depend on u through the dependence of that parameter on the rapidity functionals defined by the thermodynamic BA equations, Eqs. (107)-(110). Within the present operartor formulation, the energy eigenvalues obtained in that reference can be expressed as functionals of the occupancy configurations of the $\beta = c, \eta\nu, s\nu$ bands discrete momentum values q_j as follows,

$$\begin{aligned}
E_{symm} &= -2t \sum_{j=1}^{N_a} [N_c(q_j)\,(\cos k_c(q_j) + u) - u/2] \\
&+ 4t \sum_{\nu=1}^{\infty} \sum_{j=1}^{N_{a\eta\nu}} N_{\eta\nu}(q_j) \left[\mathrm{Re}\left\{\sqrt{1 - (\Lambda_{\eta\nu}(q_j) + i\nu\,u)^2}\right\} - \nu\,u\right].
\end{aligned} \tag{153}$$

From the interplay of symmetry with the BA solution, one can extend the results of Ref. [1] for the energy spectrum of the 1D Hubbard model in the BA solution subspace to its full Hilbert space. The energy of the unbound η-spinon and unbound spinon occupancy configurations that generate the non-LWSs corresponds to the energy terms on the right-hand side of Eq. (152) other than E_{symm}. On the other hand, the E_{symm} expression provided in Eq. (153) is valid for all 4^{N_a} energy eigenstates that span the 1D Hubbard model Hilbert space.

The limiting momentum values of Eq. (117) have simple expressions for the ground states and their excited states generated from them by occupancy-configuration deviations involving a finite number of our formulation objects. For simplicity and without loss in generality, we consider ground states with densities in the ranges $n \in [0, 1]$ and $m \in [0, n]$ for which,

$$q_c = \pi\,; \quad q_{s1} = k_{F\uparrow}\,; \quad q_{s\nu} = [k_{F\uparrow} - k_{F\downarrow}] = \pi\,m\,, \quad \nu > 1\,; \quad q_{\eta\nu} = [\pi - 2k_F] = \pi\,(1 - n)\,, \tag{154}$$

where we have ignored corrections of order $1/N_a$.

Consistent with the results of Appendix B, concerning β fermion occupancies, ground states are described by compact c and $s1$ fermion finite occupancies for momentum values in the ranges $q \in [-q_{F\beta}, +q_{F\beta}]$ where $\beta = c, s1$. On the other hand, the $\alpha\nu \neq s1$ fermion branches have vanishing ground-state occupancy. For the above ground states with densities in the ranges $n \in [0, 1]$ and $m \in [0, n]$ the c and $s1$ Fermi momenta are given by,

$$q_{Fc} = 2k_F\,; \quad q_{Fs1} = k_{F\downarrow}\,. \tag{155}$$

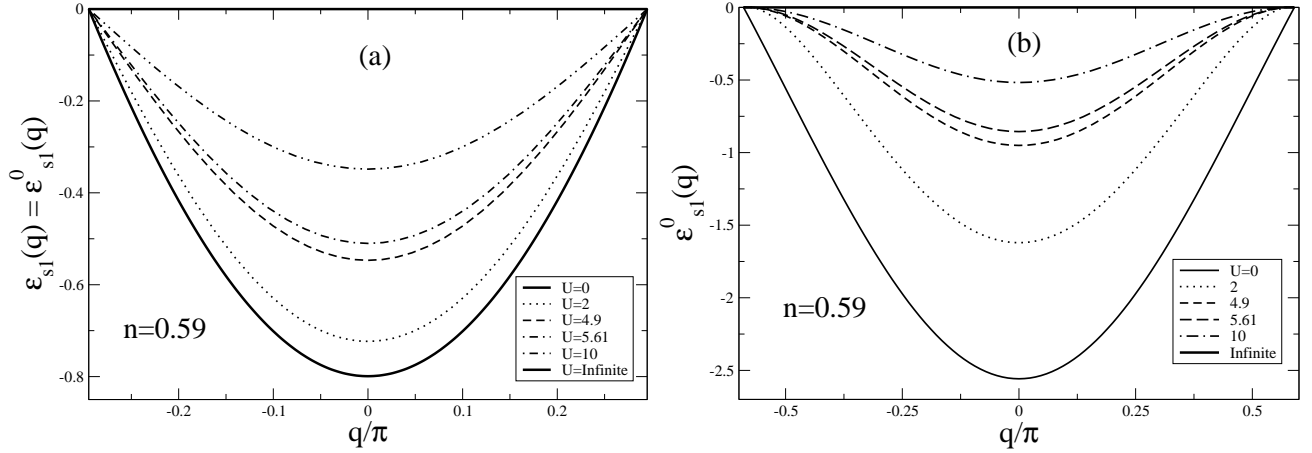Here we have again ignored corrections of order $1/N_a$.

FIG. 2: The $s1$ fermion energy dispersions $\varepsilon_{s1}(q) = \varepsilon_{s1}^0(q)$ and $\varepsilon_{s1}^0(q)$ defined by Eqs. (161) and (162) for $\beta = s1$ plotted as a function of the momentum in units of t for a set of U values (in units of t), electronic density $n = 0.59$ and (a) spin density $m = 0$ and (b) limit of maximum spin density $m \to n = 0.59$, respectively. The energy dispersions vanishing-energy ground-state energy level is marked by a horizontal line, which overlaps them at the $s1$ Fermi points $q = \pm q_{Fs1} = \pm k_F = \pm [\pi/2]\, n$ at $m = 0$ and $q = \pm q_{Fs1} = \pm 2k_F = \pm \pi n$ as $m \to n$, respectively. As discussed in the text, for general values of the spin density $m \in [0, n]$ the energy dispersion $\varepsilon_{s1}^0(q) \leq 0$ can for the absolute-value momentum range $|q| \in [q_{Fs1}, q_{s1}]$ be identified with the two-spinon binding energy within the spin-neutral $s1$ fermion. The energy dispersion $\varepsilon_{s1}^0(q) \leq 0$ plotted here in figure (b) for $m \to n = 0.59$ is thus such a binding energy.

We denote by $k_c^0(q_j)$ and $\Lambda_\beta^0(q_j)$ the rapidity-function solutions of Eqs. (107)-(109) that refer to a ground state. Those play an important role both in the PDT of Refs. [8–10] and pseudofermion scattering theory introduced in the second paper. Upon suitable manipulations of Eqs. (107)-(109), such ground-state functions $k_c^0(q_j)$ and $\Lambda_\beta^0(q_j)$ may be defined in terms of their inverse functions $q_j = q_j(\Lambda_{\beta,j}^0)$ as,

$$q_j = F_\beta^0(\Lambda_\beta^0(q_j)) + (-1)^{\delta_{\beta,\eta\nu}} \int_{-Q}^{Q} dk\, \bar{\Phi}_{c,\beta}\left(\frac{\sin k}{u}, \frac{\Lambda_\beta^0(q_j)}{u}\right), \quad j = 1, ..., N_{a_\beta},$$

$$F_c^0(\Lambda) = \arcsin(\Lambda); \quad F_c^0(\Lambda_c^0(q_j)) = k_c^0(q_j),$$
$$F_{\alpha\nu}^0(\Lambda) = \delta_{\alpha,\eta}\, 2\text{Re}\left[\arcsin(\Lambda + i\nu\, u)\right]. \tag{156}$$

Here $N_{a_\beta} = N_a$ for $\beta = c$, $N_{a_{\alpha\nu}}$ is given in Eqs. (101) and (102), the functions $\bar{\Phi}_{c,\beta}(r, r')$ are defined in the second paper, and the parameter $Q = k_c^0(2k_F)$ is the value of the ground-state rapidity function $k_c^0(q_j)$ at the c Fermi point $q_{Fc} = 2k_F$.

The β fermion momentum-distribution function deviation,

$$\delta N_\beta(q_j) = N_\beta(q_j) - N_\beta^0(q_j), \quad j = 1, ..., N_{a_\beta}, \quad \beta = c, \alpha\nu, \tag{157}$$

also plays an important role both in the PDT of Refs. [8–10] and pseudofermion scattering theory introduced in the second paper. In it, $N_\beta(q_j)$ is the excited-state β fermion momentum-distribution function. Here $N_\beta^0(q_j)$ is the initial ground-state β momentum distribution function.

Within our general notation, the momentum deviations $\delta N_\beta(q_j)$ given in Eq. (157) are labelled by the β band momentum value q_j. The corresponding β band momentum function distribution $N_\beta(q_j)$ can only have the values $N_\beta(q_j) = 1$ for occupied momentum values and $N_\beta(q_j) = 0$ for unoccupied momentum values. Therefore, the β band momentum function distribution deviation $\delta N_\beta(q_j)$ can only have the values $\delta N_\beta(q_j) = 0$, $\delta N_\beta(q_j) = -1$, and $\delta N_\beta(q_j) = +1$. Moreover, its values $\delta N_\beta(q_j) = -1$ and $\delta N_\beta(q_j) = +1$ can only occur provided that in the β band momentum function distribution $N_\beta^0(q_j)$ the corresponding discrete momentum value q_j, which may be shifted for the excited state, is occupied and unoccupied, respectively. Since for the discrete momentum values q_j for which $\delta N_\beta(q_j) = 0$ the β momentum distribution function deviation $\delta N_\beta(q_j)$ does not contribute to the excitation spectra, we need only to define it by those for which $\delta N_\beta(q_j) = -1$ and $\delta N_\beta(q_j) = +1$. (The set of β band momentum values q_j left over are then those for which $\delta N_\beta(q_j) = 0$.)

Within the present $N_a \gg 1$ limit, for simplicity we often approximate the discrete momentum values q_j by a continuum variable q. Consistent with $[q_{j+1} - q_j] = 2\pi/N_a$, in this case the above β band momentum distribution

function deviation values $\delta N_\beta(q_j) = -1$ and $\delta N_\beta(q_j) = +1$ become $\delta N_\beta(q) = -2\pi/N_a$ and $\delta N_\beta(q) = +2\pi/N_a$, respectively. The BA quantum numbers I_j^β given in Eq. (113) where $\beta = c, \alpha\nu$, $\alpha = \eta, s$, and $\nu = 1, ..., \infty$ are the β band discrete momentum values $q_j = [2\pi/N_a] I_j^\beta$ in units of $2\pi/N_a$. Depending on G_β as defined in Eq. (114) being an even or odd integer number, the quantum numbers I_j^β are integer or half-odd integers, respectively. Hence if under a transition from the ground state to an excited state the G_β value changes by an odd integer the corresponding β band discrete momentum values $q_j = [2\pi/N_a] I_j^\beta$ undergo a collective shift given by $\pm\pi/N_a$. Within the representation of the discrete momentum values q_j by a continuum variable q, such an effect is captured by deviations $\delta N_\beta(q) = \pm\pi/N_a$ for q at the β Fermi points. Those are additional possible β band momentum distribution function deviation values in addition to the above $\delta N_\beta(q) = -2\pi/N_a$ and $\delta N_\beta(q) = +2\pi/N_a$ values associated with creation of one β pseudofermion hole and one β pseudofermion of momentum q, respectively.

Consistent, the general form of the corresponding momentum distribution function deviation $\delta N_\beta(q)$ is,

$$
\begin{aligned}
\delta N_\beta(q) &= \frac{2\pi}{N_a} \sum_{p=1}^{N_\beta^p} \delta(q - q_p) - \frac{2\pi}{N_a} \sum_{h=1}^{N_\beta^h} \delta(q - q_h); \quad \text{if } \delta G_\beta \text{ even for } \beta = c, s1, \\
&= \frac{2\pi}{N_a} \sum_{p=1}^{N_\beta^p} \delta(q - q_p) - \frac{2\pi}{N_a} \sum_{h=1}^{N_\beta^h} \delta(q - q_h) \pm \frac{\pi}{N_a} \sum_{j=\pm 1} j\, \delta(q - j\, q_{F\beta}); \quad \text{if } \delta G_\beta \text{ odd for } \beta = c, s1, \\
\delta N_\beta(q) &= \frac{2\pi}{N_a} \sum_{p=1}^{N_\beta^p} \delta(q - q_p); \quad \text{for } \beta = \alpha\nu \neq s1,
\end{aligned}
\tag{158}
$$

where here and throughout this paper $\delta(x)$ denotes the usual Dirac delta-function distribution, $q_1, ..., q_{N_\beta^p}$ are the excited-state momentum values of the N_β^p added β fermions, $q_1, ..., q_{N_\beta^h}$ those of the N_β^h added β fermion holes, and δG_β stands for the deviation in the value of the number given in Eq. (114) for the $\beta = c, s1$ branches. The additional term in the expression given in Eq. (158) that emerges when the deviation δG_β is for the $\beta = c, s1$ branches a odd integer number results from the corresponding $\beta = c, s1$ band momentum shift $\pm\pi/N_a$.

For ground-state - excited-state transitions for which the number of discrete momentum values N_{a_β} changes, it is considered that the removal or addition of such values happens after the β band momentum shift, if it occurs. The removed or added discrete momentum values are always located just before the excited-state limiting momentum $-q_\beta$ or just after the excited-state limiting momentum q_β. Here q_β is given in Eq. (117) for $\beta \neq c$. For the c momentum band the limiting momentum values $q_c^\pm$ may either be symmetrical, $q_c^+ + q_c^- = 0$, or slightly asymmetrical, $q_c^+ + q_c^- = \pm 2\pi/N_a$. (We recall that such values are provided in Eqs. (B.15)-(B.17) of Ref. [21].) The order of (a) the processes involving β fermion creation or annihilation and (b) the exotic processes involving β band discrete-momentum-values addition or removal is always such that the latter processes refer to unoccupied momentum values. Hence they are zero-momentum and zero-energy processes. This is why they are not explicitly included in the β momentum distribution function deviations $\delta N_\beta(q_j)$ as defined above.

The use in the rapidity functional equations provided in Eqs. (107)-(108) and general energy spectra given in Eqs. (152) and (153) of distribution functions of form $N_\beta(q_j) = N_\beta^0(q_j) + \delta N_\beta(q_j)$ and their combined and consistent solution up to first order in the deviations $\delta N_\beta(q_j)$ given in Eq. (157), leads to the energy functionals,

$$
\delta E_{symm} = \sum_\beta \sum_{j=1}^{N_{a_\beta}} \varepsilon_\beta^0(q_j) \delta N_\beta(q_j),
\tag{159}
$$

and

$$
\begin{aligned}
\delta E &= \sum_\beta \sum_{j=1}^{N_{a_\beta}} \varepsilon_\beta(q_j) \delta N_\beta(q_j) + 2\mu\, M_{\eta,-1/2}^{un} + 2\mu_B\, H\, M_{s,-1/2}^{un}, \\
&= \sum_{\beta=c,s1} \sum_{j=1}^{N_{a_\beta}} \varepsilon_\beta(q_j) \delta N_\beta(q_j) + \sum_{\alpha\nu \neq s1} \sum_{j=1}^{N_{a_{\alpha\nu}}} \varepsilon_{\alpha\nu}^0(q_j) \delta N_{\alpha\nu}(q_j) \\
&\quad + 2|\mu|\, M_{\eta,-1/2} + 2\mu_B\, |H|\, [\delta M_{s,-1/2} - \delta N_{s1}],
\end{aligned}
\tag{160}
$$

associated with such energy spectra, respectively. The energy dispersions $\varepsilon_\beta^0(q_j)$ appearing here can be expressed in
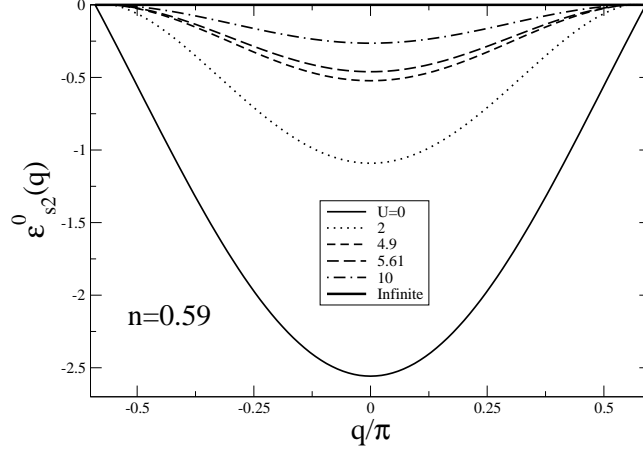
FIG. 3: The $s2$ fermion energy dispersion $\varepsilon_{s2}^0(q)$ defined by Eq. (161) for $\beta = s2$ plotted as a function of the momentum in units of t for electronic density $n = 0.59$, limit of maximum spin density $m \to n = 0.59$, and a set of U values (in units of t). The energy dispersion $u \to \infty$ limit corresponds to the vanishing-energy horizontal line. The $s2$ momentum band and corresponding energy dispersion do not exist at $m = 0$, both their momentum and energy bandwidths vanishing as $m \to 0$. The energy dispersion $\varepsilon_{s2}^0(q) \leq 0$ plotted here is the four-spinon binding energy within the spin-neutral $s2$ fermion.

terms of the initial ground-state rapidity functions $\Lambda_\beta^0(q_j)$ with $\Lambda_c^0(q_j) \equiv \sin k_c^0(q_j)$ for $\beta = c$ as follows,

$$
\begin{aligned}
\varepsilon_\beta^0(q_j) &= E_\beta^0(q_j) + 2t \int_{-Q}^{Q} dk\, \bar{\Phi}_{c,\beta}\left(\frac{\sin k}{u}, \frac{\Lambda_\beta^0(q_j)}{u}\right) \sin k\,, \quad j = 1, ..., N_{a_\beta}\,, \\
E_c^0(q_j) &= -\frac{U}{2} - 2t \cos k_c^0(q_j)\,, \\
E_{\alpha\nu}^0(q_j) &= \delta_{\alpha,\eta}\left\{-\nu U + 4t\mathrm{Re}\left[\sqrt{1 - (\Lambda_{\eta\nu}^0(q_j) + i\nu\, u)^2}\right]\right\}\,.
\end{aligned}
\tag{161}
$$

Furthermore, the energy-shifted dispersions $\varepsilon_\beta(q_j)$ are given by,

$$
\begin{aligned}
\varepsilon_c(q_j) &= \varepsilon_c^0(q_j) - \varepsilon_c^0(q_{Fc}) = \varepsilon_c^0(q_j) + (1 - \delta_{n,1})\,|\mu| + \delta_{n,1}\,\mu^0 - \mu_B\,|H|\,, \\
\varepsilon_{s1}(q_j) &= \varepsilon_{s1}^0(q_j) - \varepsilon_{s1}^0(q_{Fs1}) = \varepsilon_{s1}^0(q_j) + 2\mu_B\,|H|\,, \\
\varepsilon_{s\nu}(q_j) &= \varepsilon_{s\nu}^0(q_j) + 2\nu\mu_B\,|H|\,, \\
\varepsilon_{\eta\nu}(q_j) &= \varepsilon_{\eta\nu}^0(q_j) + (1 - \delta_{n,1})\,2\nu|\mu| + \delta_{n,1}\,2\nu\mu^0\,.
\end{aligned}
\tag{162}
$$

The functions $\bar{\Phi}_{c,\beta}(r, r')$ appearing in Eq. (161) are defined in the second paper and the inverse functions of the singled value ground-state functions $\Lambda_\beta^0(q_j)$ are defined in Eq. (156). As illustrated below in Section V F, the one- and two-electron energy excitation spectra can be expressed in terms of simple occupancies of the β fermion energy bands defined in Eqs. (161) and (162).

The standard operational formalism of second quantization can be applied to the $\alpha\nu$ fermion for transitions within the extended Takahashi subspaces, which correspond to $\alpha\nu$-band particle-hole processes. Alike for the $\alpha\nu$ bond-particle operators, the $\alpha\nu$ fermion creation or annihilation operators also play a role in transitions between different extended Takahashi subspaces, whose description is beyond the traditional operational formalism of second quantization. We note that the standard formalism does not apply only in that the transition generators cannot be expressed in terms of $\alpha\nu$ fermion creation or annihilation operators alone. However, they can be written as a product of two operators, one of which is a $\alpha\nu$ fermion creation or annihilation operator. The other operator raises or lessens the number of discrete momentum values $N_{a_{\alpha\nu}}$ of the initial subspace $\alpha\nu$ momentum band. Concerning the excitation energy spectrum though, only the processes generated by the $\alpha\nu$ fermion creation or annihilation operators play an active role. Indeed in the $N_a \to \infty$ limit raising or lessening the number of the $\alpha\nu$ band discrete momentum values is a zero-energy and zero-momentum process. This is why the $\alpha\nu$ fermion energy dispersion defined in Eqs. (161) and (162) is the bare energy for addition/removal of one $\alpha\nu$ fermion.

For electronic densities $n \neq 1$ the values of the chemical potential $\mu = \mu(n)$ and magnetic-field energy $2\mu_B H = 2\mu_B H(m)$ appearing on the right-hand side of Eq. (160), whose ranges are given in Eqs. (C1) and (C6) of Appendix
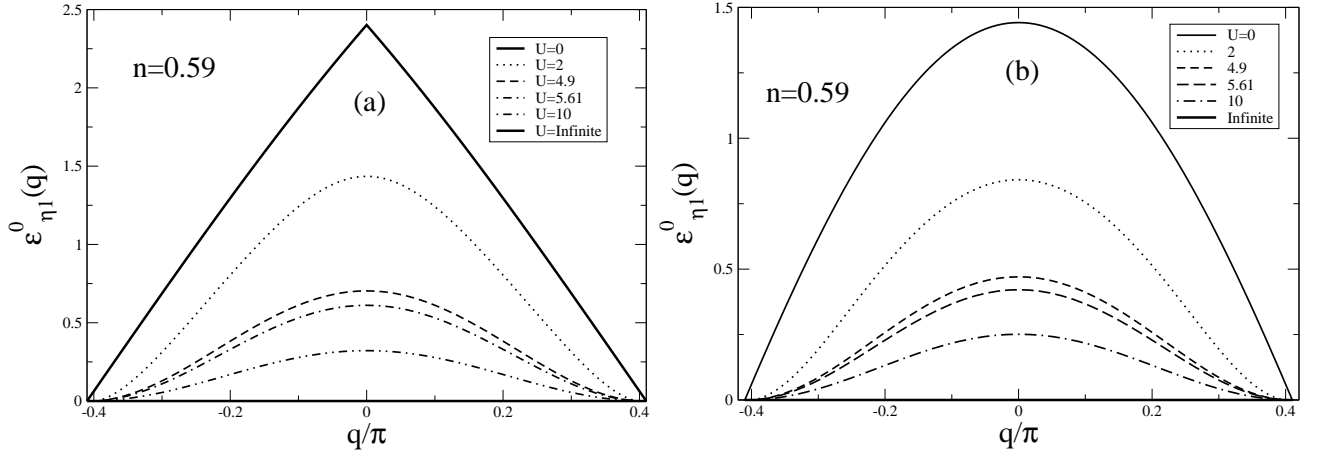
FIG. 4: The $\eta 1$ fermion energy dispersion $\varepsilon_{\eta 1}^0(q_j)$ defined by Eq. (161) for $\beta = \eta 1$ plotted in units of t for a set of U values (in units of t), electronic density $n = 0.59$, (a) spin density $m = 0$ and (b) limit of maximum spin density $m \to n = 0.59$. The energy dispersion $u \to \infty$ limit corresponds to the vanishing-energy horizontal line. The energy dispersion $\varepsilon_{\eta 1}^0(q) \geq 0$ plotted here is the two-η-spinon anti-binding energy within the η-spin-neutral $\eta 1$ fermion.

C, respectively, are fully controlled by the energy dispersions of the $\beta = c, s1$ fermion branches defined in Eq. (161). They read,

$$\mu = \mathrm{sgn}\{(1-n)\}\left[\varepsilon_c^0(q_{Fc}) + \frac{1}{2}\varepsilon_{s1}^0(q_{Fs1})\right] ; \quad 2\mu_B H = \mathrm{sgn}\{m\}\varepsilon_{s1}^0(q_{Fs1}), \quad n \neq 1 . \tag{163}$$

The expressions given here are valid for the whole range of densities $n \neq 1$ and m.

The energy functional of Eq. (160) includes interaction terms, which are of second order in the deviations $\delta N_\beta(q_j)$, beyond those given in that equation. Such terms correspond to $1/N_a$ corrections to the energy functional provided in Eq. (160). Due to the occurrence of an infinite set of conservation laws associated with the model integrability in the BA solution subspace [41–43, 54], such interactions are of zero-momentum forward-scattering type. Such second-order in the deviations $\delta N_\beta(q_j)$ interaction energy terms and related dressed phase shifts, dressed S matrix, and scattering theory are issues studied in the second paper.

The energy dispersions $\varepsilon_c(q)$, $\varepsilon_{s1}(q)$ and $\varepsilon_{s1}^0(q)$, $\varepsilon_{s2}^0(q)$, $\varepsilon_{\eta 1}^0(q)$, and $\varepsilon_{\eta 2}^0(q)$ are plotted as a function of the momentum q in Figs. 1, 2, 3, 4, and 5, respectively, for several U/t values, and electronic density $n = 0.59$. The two dispersions plotted in each of the Figs. 1, 2, 4, and 5 refer to the spin-density limits $m \to 0$ and $m \to n = 0.59$, respectively. In the $m \to 0$ limit the momentum and energy bandwidths of the $s2$ fermion energy dispersion vanish, so that in Fig. 3 it is plotted only for the spin-density limit $m \to n = 0.59$. For $m = 0$ the electronic density $n = 0.59$ is that used in the studies of Ref. [11] of the photoemission spectrum of the quasi-1D metal TTF- TCNQ. The figures U/t values are $U/t = 0, 2, 4.9, 5.61, 10, \infty$. Here $U/t = 4.9$ and $U/t = 5.6$ are the values suitable to the spectral lines of the TCNQ and TTF molecular stacks, respectively, in the investigations of Ref. [11].

Limiting expressions of the energy dispersions $\varepsilon_c(q)$, $\varepsilon_{s1}(q)$, and $\varepsilon_{\eta\nu}^0(q)$ corresponding to $u \to 0$ and $u \gg 1$ are given in Eqs. (C12)-(C14) of Appendix C for electronic density $n \in [0, 1]$ and spin density $m = 0$. In the maximum spin-density limit, $m \to n$, all β fermion energy dispersions have simple closed-form expressions. Those are given Eqs. (C15)-(C16) of Appendix C. In that limit the ground-state $s1$ band momentum limiting values read $\pm q_{s1} = \pm k_{F\uparrow} = \pm 2k_F = \pm\pi n$ and have the same values as those of the remaining ground-state $s\nu$ band momentum limiting values, $\pm q_{s\nu} = \pm[k_{F\uparrow} - k_{F\downarrow}] = \pm 2k_F = \pm\pi n$. On the other hand, the ground-state $\eta\nu$ band momentum limiting values are in that limit given by their general n dependent expression $\pm q_{\eta\nu} = \pm[\pi - 2k_F] = \pm\pi[1 - n]$.

The corresponding $\alpha\nu$ fermion dispersion energy bandwidths are given by,

$$W_{\alpha\nu} = |\varepsilon_{\alpha\nu}^0(q_{\alpha\nu}) - \varepsilon_{\alpha\nu}^0(0)| = |\varepsilon_{\alpha\nu}^0(0)| ; \quad W_c = 4t . \tag{164}$$

The c fermion energy dispersion bandwidth, $W_c = 4t$, is independent of n, m, and u. On the other hand, from manipulations of Eqs. (161) and (162) we find that for $\alpha\nu \neq s1$ branches the $\alpha\nu$ fermion energy dispersion bandwidths can be expressed in terms of the unbound η-spinon ($\alpha = \eta$) and unbound spinon ($\alpha = s$) energy scale $[\varepsilon_{\alpha,+1/2} + \varepsilon_{\alpha,-1/2}]$ given in Eqs. (90) and (91) as follows,

$$W_{\alpha\nu} = i_{\alpha\nu}[\varepsilon_{\alpha,+1/2} + \varepsilon_{\alpha,-1/2}]; \quad 0 \leq i_{\eta\nu} \leq 1, \quad \alpha\nu \neq s1, \quad \alpha = \eta, s . \tag{165}$$
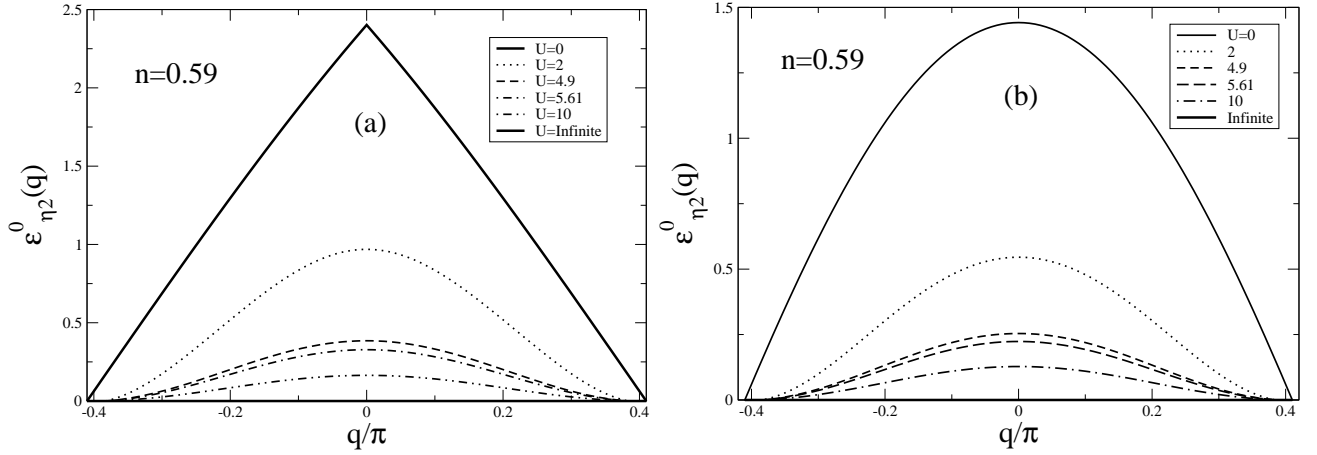
FIG. 5: The $\eta2$ fermion energy dispersion $\varepsilon^0_{\eta2}(q_j)$ defined by Eq. (161) for $\beta = \eta2$ plotted in units of t for a set of U values (in units of t), electronic density $n = 0.59$, and (a) spin density $m = 0$ and (b) limit of maximum spin density $m \to n = 0.59$. The energy dispersion $u \to \infty$ limit corresponds to the vanishing-energy horizontal line. The energy dispersion $\varepsilon^0_{\eta2}(q) \geq 0$ plotted here is the four-η-spinon anti-binding energy within the η-spin-neutral $\eta2$ fermion.

For a ground state with densities $n \in [0, 1]$ the number $i_{\alpha\nu}$ appearing here decreases continuously for increasing values of u. For $\alpha = \eta$ it has the limiting behaviors $i_{\eta\nu} \to 1$ for $u \to 0$ and $i_{\eta\nu} \to 0$ for $u \to \infty$. On the other hand, for $\alpha = s$ and $\nu > 1$ it has the limiting values $i_{s\nu} \to 1$ for $u \to 0$ and $i_{s\nu} \to 1/\nu$ for $u \to \infty$.

For a ground state with densities $n \in [0, 1]$ and $m \in [0, n]$ the corresponding $s1$ band is unoccupied for $|q| \in [k_{F\downarrow}, k_{F\uparrow}]$ and occupied for $|q| \in [0, k_{F\downarrow}]$. Again from the use of Eqs. (161) and (162), we find that the $s1$ energy bandwidth W_{s1} defined in Eq. (164) can for $\alpha\nu = s1$ be expressed as,

$$
\begin{aligned}
W_{s1} &= W^h_{s1} + W^p_{s1}; \quad W^h_{s1} = [\varepsilon_{s1}(k_{F\uparrow}) - \varepsilon_{s1}(k_{F\downarrow})]; \quad W^p_{s1} = [\varepsilon_{s1}(k_{F\downarrow}) - \varepsilon_{s1}(0)], \\
W^h_{s1} &= [\varepsilon_{s,+1/2} + \varepsilon_{s,-1/2}] = 2\mu_B |H|.
\end{aligned}
\tag{166}
$$

Here W^h_{s1} and W^p_{s1} are the energy bandwidths of the ground-state $s1$ fermion hole and $s1$ fermion seas, respectively. For the electronic density range $n \in [0, 1]$, their limiting behaviors are $W^h_{s1} \to 0$ for $m \to 0$, $W^h_{s1} \to W_{s1}$ for $m \to n$, $W^p_{s1} \to W_{s1}$ for $m \to 0$, and $W^p_{s1} \to 0$ for $m \to n$.

For $n \in [0, 1]$ and $m \to n$ the energy bandwidths $W_{s\nu}$ and $W_{\eta\nu}$ have closed-form expressions, provided in Eqs. (C17)-(C20) of Appendix C. At $n = 1$ and $m = 0$ the $W_{s1} = W^p_{s1}$ bandwidth u dependence is for the whole $u > 0$ range given in Eq. (C21) of that Appendix. The behaviors for both $u \to 0$ and $u \to \infty$ of the energy bandwidths $W_{s\nu}$ and $W_{\eta\nu}$ are reported in Eqs. (C22) and (C23) of Appendix C for electronic densities $n \in [0, 1]$ and both spin densities $m = 0$ and $m \to n$. That such energy bandwidths vanish as $u \to \infty$ follows from all spin and η-spin configurations being degenerate in that limit. In the limits $n \to 1$ and $m \to 0$ the $\eta\nu$ bands and $\nu > 1$ $s\nu$ bands collapse into the point $\varepsilon^0_{\eta\nu}(0) = 0$ and $\varepsilon^0_{s\nu}(0) = 0$, so that $W_{\eta\nu} \to 0$ and $W_{s\nu} \to 0$, respectively.

The BA solution performs the sum of all Hamiltonian terms on the right-hand side of both Eqs. (72) and (73) and beyond. The corresponding expression of the 1D Hubbard model Hamiltonian $\hat{H}_{symm}$ appearing in such equations and in Eqs. (1) and (2) is simply obtained by replacing the β fermion numbers $N_\beta(q_j)$, rapidity momentum functions $k_c(q_j)$, and rapidity functions $\Lambda_{\alpha\nu}(q_j)$ in the general energy expression of Eq. (153) by the corresponding β fermion number operators, c rapidity momentum operators, and $\alpha\nu$ rapidity operators, respectively. This gives,

$$
\begin{aligned}
\hat{H}_{symm} = & -2t \sum_{j=1}^{N_a} \left[\hat{N}_c(q_j) \left(\cos \hat{k}_c(q_j) + u \right) - u/2 \right] \\
& + 4t \sum_{\nu=1}^{\infty} \sum_{j=1}^{N_{a\eta\nu}} \hat{N}_{\eta\nu}(q_j) \left[\text{Re} \left\{ \sqrt{1 - (\hat{\Lambda}_{\eta\nu}(q_j) + i\nu\,u)^2} \right\} - \nu\,u \right].
\end{aligned}
\tag{167}
$$

As discussed above, the c rapidity momentum operators and $\alpha\nu$ rapidity operators are implicitly defined by the thermodynamic BA equations, Eqs. (107)-(109).

F.   Simple excitations spectra in terms of the c and $s1$ fermion energy dispersions

The one- and two-electron excited states mostly considered in the vast literature of the 1D Hubbard model are those of an initial ground state with electronic density in the range $n \in [0,1]$ and vanishing spin density, $m = 0$. The energy spectrum of such excited states has simple expressions in terms of the c and $s1$ energy dispersions defined in Eq. (162). Here we revisit some of such excited states. One of our aims is to describe the microscopic processes that generate such states in terms of the elementary objects of our operational formulation. The corresponding spectra are expressed in terms of such objects energy dispersions.

Consistent with the results of Appendix B, that $m = 0$ ground-state occupancies of the objects of our formulation are,

$$
\begin{aligned}
M_s &= M_s^{bo} = N = n\, N_a \,; \quad M_s^{bo} = N \,; \quad M_{s,\pm 1/2}^{un} = 0 \,, \\
M_\eta &= M_\eta^{un} = M_{\eta,+1/2}^{un} = N_a - N = (1-n)\, N_a \,, \\
N_c &= N \,; \quad N_{s1} = N/2 \,; \quad N_{s1}^h = 0 \,.
\end{aligned}
\tag{168}
$$

For simplicity, we consider that $N/2$ is an odd integer number, so that $N_c = N$ and $N_{s1} = N/2$ are even and odd integer numbers, respectively. Such a $m = 0$ ground state has no unbound spinons and no $s1$ fermion holes, $M_s^{un} = 0$ and $N_{s1}^h = 0$, respectively. For it all $s1$ band momenta $q \in [-q_{Fs1}, +q_{Fs1}] = [-k_F, +k_F]$ where $k_F = \pi n/2$ are occupied. Moreover, the c band momenta are occupied for $q \in [-q_{Fc}, q_{Fc}] = [-2k_F, 2k_F]$ and unoccupied for $|q| \in [q_{Fc}, q_c] = [2k_F, \pi]$ where $2k_F = \pi n$. Here we have ignored $1/N_a$ order corrections, which vanish within the thermodynamic limit. The $\mu = 0$, $n = 1$, and $m = 0$ absolute ground state is a particular case of the $m = 0$ ground state for which the number values of Eq. (168) apply with $n = 1$ and thus $N = N_a$. For the absolute ground state the c band is full and there are no unbound η-spinons.

The $N_{s1}^h = 2$ spin-singlet excited states of such a $m = 0$ and $N_{s1}^h = 0$ ground state have deviations given by,

$$
\begin{aligned}
\delta N_c &= -\delta M_{\eta,+1/2}^{un} = 0 \,; \quad \delta N_{s1} = -2 \,; \quad \delta N_{s1}^h = N_{s1}^h = 2 \,; \quad \delta N_{s2} = N_{s2} + 1 \,, \\
&\pm \pi/L \; -c-\text{band}-\text{momentum}-\text{shift} \,.
\end{aligned}
\tag{169}
$$

The number values of such excited energy eigenstates are the sum of those of the corresponding initial $m = 0$ ground state provided in Eq. (168) plus their deviations given here. Nearly all the spectral weight associated with the spin-singlet excitations is originated by the processes associated with such deviations. Within the ground-state transitions to such excited energy eigenstates, the c band momentum values undergo alternative collective shifts, $\pm \pi/L$. Those lead to a macroscopic momentum contribution given by $\pm 2k_F = \pm \pi n$. Within such transitions, the number of annihilated $s1$ fermions exactly equals that of holes emerging in the $s1$ band, so that the number of discrete momentum values $N_{a_{s1}}$ is preserved.

Under such $N_{s1}^h = 2$ spin-singlet excitations the spinon pairs of the two annihilated $s1$ fermions are broken. The four spinons left over reorganize in the final excited state within a spin-singlet four-spinon composite $s2$ fermion configuration. The emerging composite $s2$ fermion has vanishing momentum, energy, binding energy, and velocity. Its $s2$ effective lattice is reduced to a single occupied site, which corresponds to four sites of the underlying spin effective lattice.

The spectrum of such spin-singlet excited states is degenerate with that of the spin-triplet excited states, whose deviations are given by,

$$
\begin{aligned}
\delta N_c &= -\delta M_{\eta,+1/2}^{un} = 0 \,; \quad \delta N_{s1} = -1 \,; \quad \delta N_{s1}^h = N_{s1}^h = 2 \,; \quad \delta M_s^{un} = M_s^{un} = 2 \,, \\
&\pm \pi/L \; -c-\text{band}-\text{momentum}-\text{shift} \,, \\
&\mp \pi/L \; -s1-\text{band}-\text{momentum}-\text{shift} \,.
\end{aligned}
\tag{170}
$$

Nearly all the spectral weight associated with the spin-triplet excitations is originated by the processes associated with such deviations, which generate exact energy eigenstates. The c and $s1$ band momentum alternative collective shifts $\pm \pi/L$ and $\mp \pi/L$, respectively, result here from the changes in the boundary conditions that determine the integer of half-odd integer values of the BA c and $s1$ quantum numbers, Eq. (113). Those of the c band lead to a macroscopic momentum contribution given by $\pm 2k_F = \pm \pi n$. On the other hand, the $s1$ band momenta collective shifts $\pm \pi/L$ generate a macroscopic momentum $\pm k_F = \pm \pi n/2$. For the lowest-energy states of such an excitation branch that microscopic momentum exactly cancels another momentum contribution, $\mp k_F = \mp \pi n/2$. The latter momentum arises from the emergence of a hole at $s1$ band momentum $q = \pm k_F = \pm \pi n/2$, due to the $s1$ fermion removal. Therefore, the $s1$ band momentum collective shifts do not lead to any net momentum contribution in the general spin spectrum given below.
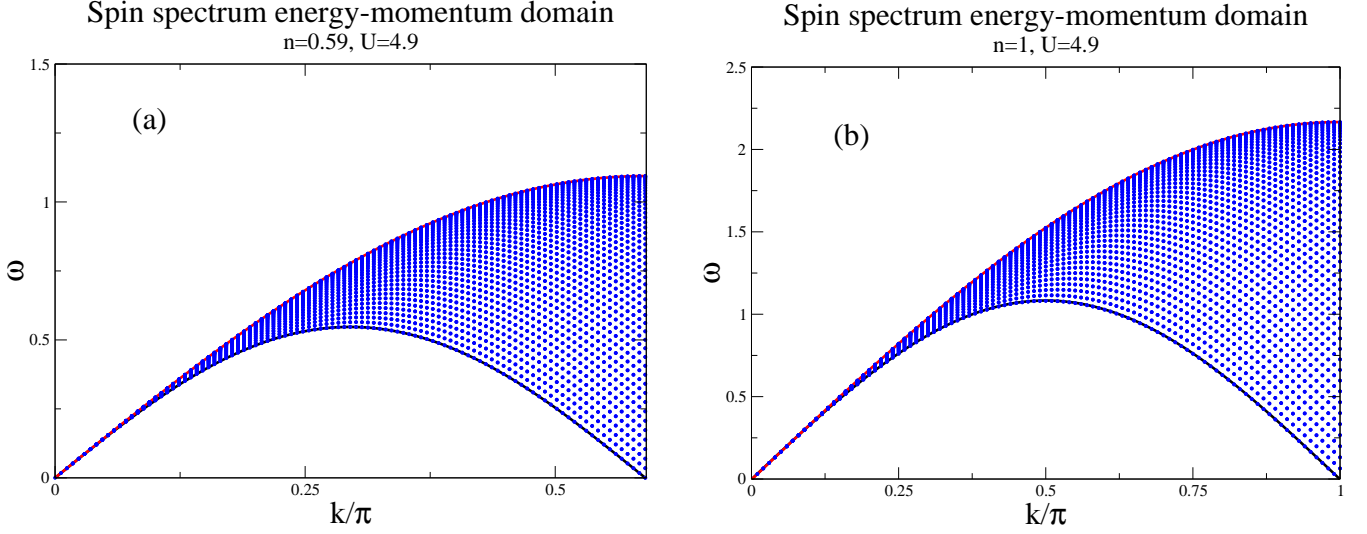
FIG. 6: The (k,ω) plane domain of the spin spectrum of Eq. (171) with the energy in units of t for $U/t = 4.9$, spin density $m = 0$, and electronic densities (a) $n = 0.59$ and (b) $n = 1$. The shape of this spin spectrum is determined by the occupancy configurations of two holes in the $s1$ fermion energy dispersion plotted in Fig. 2 (a).

A second $s1$ band hole appears at the opposite $s1$ band limiting side, due to the emergence of a discrete momentum value, which is associated with the deviation $\delta N_{a_{s1}} = [\delta N_{s1} + \delta N_{s1}^h] = 1$. This process does not generate any momentum but drives the system into a virtual unphysical state whose $s1$ band limits are not symmetrical. For all 4^{N_a} energy eigenstates the $\alpha\nu$ momentum bands are symmetrical around zero, with the limiting momentum values reading $\pm q_{\alpha\nu}$ where $q_{\alpha\nu}$ is given in Eq. (117). The above $s1$ band momentum collective shift $\pm\pi/L$ restores that symmetry and leads to the final physical state. (Actually, all such processes cannot be separated, so that the virtual state is an artifact of our separation of the overall process into intermediate virtual processes.)

In contrast to the $N_{s1}^h = 2$ spin-singlet excited states, the number of discrete momentum values $N_{a_{s1}}$ of the spin-triplet states is not preserved. However, since for the spin-singlet excited states there is no $s1$ band momentum collective shift, in the thermodynamic limit their energy and momentum spectra are exactly the same. Both the transitions from the initial $m = 0$ ground state to the spin-singlet and spin-triplet excited energy eigenstates whose number deviations are given in Eqs. (169) and (170) involve the emergence of two holes in the $s1$ fermion band. (The spin weight originated by four-$s1$-band-hole excited energy eigenstates is very small for u finite and vanishes as $u \to \infty$.)

The degenerate spectrum of the $N_{s1}^h = 2$ spin-singlet and spin-triplet excited states can be expressed as,

$$
\begin{aligned}
\omega(k) &= -\varepsilon_{s1}(q) - \varepsilon_{s1}(q'); \quad k = [\pm 2k_F - q - q'] = [\pm\pi\, n - q - q'], \\
q, q' &\in [-k_F, k_F] = [-\pi\, n/2, \pi\, n/2].
\end{aligned}
\tag{171}
$$

Its (k,ω) plane domain is represented in Fig. 6 for $U/t = 4.9$, spin density $m = 0$, and electronic densities (a) $n = 0.59$ and (b) $n = 1$. It is generated by all two-hole $s1$ band occupancy configurations of the $s1$ fermion energy dispersion plotted in Fig. 2 (a).

The number and deviation values given in Eq. (170) apply to the three branches of spin-triplet excited states. For that inside the BA solution subspace the excited-state unbound-spinon number $\delta M_s^{un} = M_s^{un} = 2$ refers to $M_{s,+1/2}^{un} = 2; M_{s,-1/2}^{un} = 0$. The remaining two spin-triplet excited state branches are outside the BA solution subspace, yet are accounted for by the present operator formulation. Specifically, they have unbound-spinon numbers $M_{s,+1/2}^{un} = 1; M_{s,-1/2}^{un} = 1$ and $M_{s,+1/2}^{un} = 0; M_{s,-1/2}^{un} = 2$, respectively, and are generated from the corresponding $M_{s,+1/2}^{un} = 2; M_{s,-1/2}^{un} = 0$ spin-triplet excited state inside that subspace by spin-flipping one and two unbound spinons, respectively.

Finally, we consider the simplest one-electron excited states of the $\mu = 0$, $n = 1$, and $m = 0$ absolute ground state. Within our rotated-electron operational description, the one-electron lower-Hubbard-band (LHB) and upper-Hubbard-band (UHB) are well-defined concepts. Specifically, the one-electron LHB is generated by transitions from a $n < 1$ (and $n > 1$) ground state to excited energy eigenstates with no rotated-electron doubly occupied sites (and no rotated-electron unoccupied sites). For an initial $n = 1$ ground state such transitions do not exist. The first UHB is

generated by transitions from $n \leq 1$ (and $n \geq 1$) ground states to excited energy eigenstates with one rotated-electron doubly occupied site (and one rotated-electron unoccupied site). For one-electron addition excitations, the spectral weight generated by transitions to excited energy eigenstates with two rotated-electron doubly occupied sites is very small. Those transitions generate the second UHB.

Here we discuss only the case of the one-electron addition first UHB of the initial $\mu = 0$ Mott-Hubbard-insulating absolute ground state. By simplicity, we call UHB the first UHB. A selection rule prevents the occurrence of one-electron addition excited states involving creation of $\eta\nu$ fermions onto that ground state. Indeed, the corresponding $\delta N = 1$ deviation is in that case given by $\delta N = [\delta N_c + \sum_{\nu=1}^{\infty} 2\nu \delta N_{\eta\nu}] = 1$. On the other hand, the corresponding deviation in the η-spin value reads $\delta S_\eta = -\frac{1}{2}[\delta N_c + \sum_{\nu=1}^{\infty} 2\nu \delta N_{\eta\nu}] = -\frac{1}{2}$. Since $S_\eta \geq 0$, the latter deviation is only allowed for initial ground states whose η-spin value obeys the inequality $S_\eta \geq 1/2$. The one-electron addition UHB of the the $\mu = 0$ absolute ground state is generated under creation onto it of one unbound η-spinon of η-spin projection $-1/2$, which is an allowed process.

The number values of the Mott-Hubbard insulator $m = 0$, $n = 1$, and $\mu = 0$ absolute ground state are those provided in Eq. (168) for $N = N_a$. The UHB one-electron addition spectral weight associated with the creation of one rotated-electron doubly occupied site onto that state is generated by processes whose number deviations are given by,

$$\delta N_c = -1; \quad \delta N_{s1} = -1; \quad \delta N_{s1}^h = 1; \quad \delta M_{\eta,+1/2}^{un} = 0; \quad \delta M_{\eta,-1/2}^{un} = 1,$$
$$\pm\pi/L \quad -c - \text{band} - \text{momentum} - \text{shift}. \tag{172}$$

The ground-state transitions to such excited states involve a collective momentum shift $\pm\pi/L$ in the c band. Since the initial ground state is a half-filled state, the lattice translational symmetry is explicit. Thus the momentum shifts $+\pi/L$ and $-\pi/L$ lead in this case to the same c band occupancy configuration. The macroscopic momentum $\pm\pi$ generated by such a momentum shift is exactly cancelled by the momentum $\pm\pi$ of the created $-1/2$ unbound η-spinon.

The corresponding energy gapped spectrum shape is determined by the emergence of one hole in the c momentum band, one hole in the $s1$ momentum band, and the creation of one unbound η-spinon of η-spin projection $-1/2$. It reads,

$$\omega(k) = \varepsilon_{\eta,-1/2} - \varepsilon_c(q) - \varepsilon_{s1}(q'); \quad k = [-q - q']; \quad q \in [-\pi, \pi]; \quad q' \in [-\pi/2, \pi/2]. \tag{173}$$

Since the initial ground state refers to vanishing chemical potential $\mu = 0$, the unbound η-spinon energy is $\varepsilon_{\eta,-1/2} = \mu^0$, as given in Eq. (88). The creation of the $-1/2$ unbound η-spinon and corresponding rotated-electron doubly occupied site is behind the spectrum being gapped.

The $N + 1 = N_a + 1$ ground states are among the excited states whose number deviations are given in Eq. (173). They are generated by processes under which the c fermion hole and $s1$ fermion hole are created at a c Fermi points $q = \mp\pi$ and $s1$ band limiting momentum values $q' = \pm\pi/2$, respectively. In that case the general spectrum given in Eq. (173) simplifies to $\omega(k) = \varepsilon_{\eta,-1/2} = \mu^0$ and $k = \pm\pi/2 = \pm k_F$. The (k, ω) plane domain of the UHB one-electron addition spectrum provided in Eq. (173) is represented in Fig. 7. The figure refers to a reduced-zone scheme for spin density $m = 0$, electronic density $n = 1$, and (a) $U/t = 4.9$ and (b) $U/t = 13.6$.

G. Confirmation of the anti-binding η-spinon ($\alpha = \eta$) binding spinon ($\alpha = s$) character of the composite $\alpha\nu$ fermions from analysis of their energy dispersion

The unbound η-spinons and unbound spinons whose energies are given in Eqs. (87), (88), and (89) have no energy dispersion. They neither interact among themselves nor with the β fermions. In the second paper it is confirmed that unbound η-spinons and unbound spinons are neither scatterers nor scattering centers. The energies of such unbound objects play an important role as reference energy scales for the energies of the 2ν-η-spinon composite $\eta\nu$ fermions and 2ν–spinon composite $s\nu$ fermions.

The unbound η-spinon and unbound spinon energies of Eqs. (87), (88), and (89) and the energy dispersions $\varepsilon_{\eta\nu}(q)$ and $\varepsilon_{s\nu}(q)$ of Eq (162) alike are measured relative to the zero-energy level of the Hamiltonian $\hat{H}$ of Eq. (1), which is that of the initial ground state. The zero-energy level of the energy dispersions $\varepsilon_{s\nu}^0(q)$ and $\varepsilon_{\eta\nu}^0(q)$ of Eq. (161) corresponds in turn to that of the Hamiltonian $\hat{H}_{symm}$ of Eq. (2). Relative to it, the corresponding unbound spinon and unbound η-spinon energies read,

$$\varepsilon_{\alpha,\pm1/2}^0 = 0, \quad \alpha = \eta, s. \tag{174}$$

One-electron UHB addition spectrum domain
n=1, U=4.9

(a)
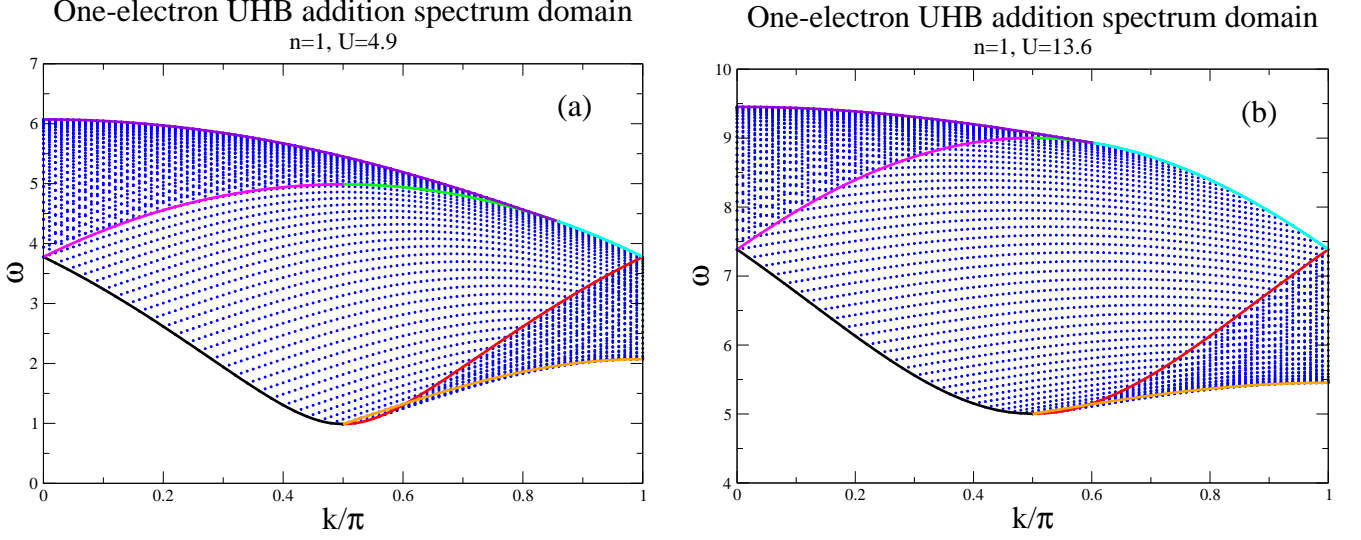
One-electron UHB addition spectrum domain
n=1, U=13.6

(b)

FIG. 7: The (k,ω) plane domain of the UHB one-electron spectrum of Eq. (173) within a reduced-zone scheme with the energy in units of t for spin density $m = 0$, electronic density $n = 1$, and (a) $U/t = 4.9$ and (b) $U/t = 13.6$. The shape of this spectrum is determined by the combined one-hole occupancy configurations of the c and $s1$ fermion energy dispersions plotted in Figs. 1 and 2 (a), respectively, plus the finite energy associated with creation of one $-1/2$ unbound η-spinon. The latter energy is behind the spectrum being gapped and refers to creation of one rotated-electron doubly occupied site.

On the other hand, relative to the zero-energy level of the initial ground state the $\eta\nu$ and $s\nu$ fermion energy dispersions are such that,

$$
\begin{aligned}
\min \varepsilon_{\eta\nu}(q) &= \varepsilon_{\eta\nu}(\pm q_{\eta\nu}) = \nu[\varepsilon_{\eta,+1/2} + \varepsilon_{\eta,-1/2}] = (1 - \delta_{n,1})\, 2\nu|\mu| + \delta_{n,1}\, 2\nu\mu^0\,, \\
\max \varepsilon_{s\nu}(q) &= \varepsilon_{s\nu}(\pm q_{s\nu}) = \nu[\varepsilon_{s,+1/2} + \varepsilon_{s,-1/2}] = 2\nu\mu_B\,|H|\,.
\end{aligned}
\tag{175}
$$

This confirms the anti-binding and binding character of the 2ν-η-spinon and 2ν-spinon occupancy configurations of a composite $\eta\nu$ fermion and composite $s\nu$ fermion, respectively. The energy scales on the right-hand side of the two equations given here are exactly $\nu = 1, ..., \infty$ times larger than the energy of a unbound η-spinon pair (and unbound spinon pair), which is provided in Eq. (87) (and Eq. (91)). That the minimum (and maximum) magnitude of the energy dispersion $\varepsilon_{\eta\nu}(q)$ (and $\varepsilon_{s\nu}(q)$) is reached at the limiting momentum values $\pm q_{\eta\nu}$ (and $\pm q_{s\nu}$) is below found to be related to important $\eta\nu$ fermion (and $s\nu$ fermion) symmetries.

The inequalities given in Eq. (175) are consistent with the behavior of the energy dispersions plotted in Figs. 2, 3, 4, and 5. For $m = 0$ and $H = 0$, the two energy dispersions $\varepsilon_{s1}(q)$ and $\varepsilon_{s1}^0(q)$ have the same zero-energy level, so that $\varepsilon_{s1}(q) = \varepsilon_{s1}^0(q)$. They are plotted in Fig. 2 (a). On the other hand, for $m \neq 0$ such two energy dispersions are as given in Eq (162) related as $\varepsilon_{s1}(q) = \varepsilon_{s1}^0(q) + 2\mu_B|H|$. Hence the zero-energy level of the energy dispersion $\varepsilon_{s1}^0(q)$ plotted in Fig. 2 (b) for $m \rightarrow n = 0.59$ and $H = H_c$ corresponds to the energy $2\mu_B H_c$ of the dispersion $\varepsilon_{s1}(q)$. Zero and $2\mu_B H_c$ are the maximum two-spinon $s1$ fermion energies of such dispersions, respectively. Moreover, the zero-energy level of the $s2$ fermion energy dispersion plotted in Fig. 3 for $m \rightarrow n = 0.59$ and $H = H_c$ corresponds to the energy $4\mu_B H_c$ of the dispersion $\varepsilon_{s2}(q)$. That is the maximum four-spinon $s2$ fermion energy of that dispersion. The zero-energy levels of the $\eta1$ and $\eta2$ fermion energy dispersions plotted in Figs. 4 and 5 correspond to the energies $2|\mu|$ and $4|\mu|$ of the dispersions $\varepsilon_{\eta1}(q)$ and $\varepsilon_{\eta2}(q)$, respectively.

The *binding energy* of one $s\nu$ fermion with $\nu > 1$ spinon pairs vanishes at the $s\nu$ band limiting momentum values $q = \pm q_{s\nu}$. Its maximum magnitude is reached at $q = 0$ and thus vanishing velocity $v_{s\nu}(q) = 0$. At $q = \pm q_{s\nu}$ the $s\nu$ fermion velocity also vanishes, $v_{s\nu}(\pm q_{s\nu}) = 0$. Relative to its energy at such limiting momentum values there is at $q = 0$ an energy gain of $-W_{s\nu}$. That energy gain equals the maximum binding energy.

It is useful for the definition of the binding energy at arbitrary $s\nu$ band momentum values $q \in (-q_{s\nu}, q_{s\nu})$ to consider a $s\nu$ fermion dispersion $\varepsilon_{s\nu}^k(q) = [\varepsilon_{s\nu}^0(q) + W_{s\nu}]$. Its zero-energy level coincides with that of the momentum $q = 0$. For small q values that energy plays the role of $s\nu$ fermion kinetic energy. At small q the $s\nu$ fermion acquires a finite velocity, $v_{s\nu}(q)$. The corresponding energy $\varepsilon_{s\nu}^k(q)$ is an increasing function of $|q|$. Its maximum magnitude is reached at $\pm q_{s\nu}$, exactly when the binding energy vanishes. Out of the two terms of the energy $\varepsilon_{s\nu}^k(q) = [\varepsilon_{s\nu}^0(q) + W_{s\nu}]$, the energy dispersion $\varepsilon_{s\nu}^0(q)$ plays the role of binding energy. As mentioned above, its absolute value is maximum at rest when $q = 0$, $v_{s\nu}(q) = 0$, and $\varepsilon_{s\nu}^0(0) = -W_{s\nu}$. For small q values, part of the $s\nu$ fermion binding energy is transferred

over to the kinetic energy $\varepsilon_{s\nu}^k(q) = [\varepsilon_{s\nu}^0(q) + W_{s\nu}]$, which becomes finite. The amount of transferred energy exactly equals the decrease in the energy scale $|\varepsilon_{s\nu}^0(q)|$ absolute value. Such an energy transfer occurs as well for larger q values, although for them the energy $\varepsilon_{s\nu}^k(q)$ is not anymore a free-like kinetic energy. When the energy $\varepsilon_{s\nu}^k(q)$ reaches its maximum magnitude, $W_{s\nu}$, at $q = \pm q_{s\nu}$ all the binding energy has been used up.

The binding energy of one $s1$ fermion created onto a ground state may also be identified with the energy scale $\varepsilon_{s1}^0(q)$. However, due to the finite $s1$ fermion ground-state occupancy, this refers now only to the $s1$ fermion-hole $s1$ band momentum ranges $q \in [-q_{s1}, -q_{Fs1}]$ and $q \in [q_{Fs1}, q_{s1}]$. At the $s1$ band Fermi points $q = \pm q_{Fs1}$ it reaches its maximum absolute value, $W_{s\nu}^h$. For $|q| \in [q_{Fs1}, q_{s1}]$ it is a decreasing function of $|q|$, vanishing at $q = \pm q_{s1}$. A similar analysis reveals that for the $\eta\nu$ fermions the *anti-binding energy* can be identified with the energy scale $\varepsilon_{\eta\nu}^0(q)$. The arguments involve now energy losses rather than gains. That energy vanishes at $q = \pm q_{\eta\nu}$. Its maximum value, $W_{\eta\nu}$, is reached at $q = 0$.

Hence the energy dispersions $\varepsilon_{\eta\nu}^0(q)$ and $\varepsilon_{s\nu}^0(q)$ defined in Eq. (161), whose zero-energy level refers to that of the Hamiltonian $\hat{H}_{symm}$ of Eq. (2), have a well defined physical meaning. Consistent with the above analysis, upon combining the unbound η-spinon and unbound spinon energy-scales expressions given in Eqs. (90) and (91), respectively, with such energy dispersions expressions provided in Eq. (162), one finds that they can be written as,

$$
\begin{aligned}
\varepsilon_{\eta\nu}^0(q) &= \varepsilon_{\eta\nu}(q_j) - \nu\left[\varepsilon_{\eta,-1/2} + \varepsilon_{\eta,+1/2}\right] \geq 0\,, \\
\varepsilon_{s\nu}^0(q) &= \varepsilon_{s\nu}(q_j) - \nu\left[\varepsilon_{s,-1/2} + \varepsilon_{s,+1/2}\right] \leq 0\,.
\end{aligned}
\tag{176}
$$

The maximum absolute value of the anti-binding energy ($\alpha = \eta$) or binding energy ($\alpha = s$) of one $\alpha\nu$ fermion created onto a ground state is the energy bandwidth of that state unoccupied $\alpha\nu$ momentum-band sea, $W_{\alpha\nu}^h$. This holds for creation of one $s1$ fermion. For the $\alpha\nu \neq s1$ branches this follows from the equality $W_{\alpha\nu} = W_{\alpha\nu}^h$. A related quantity of physical interest is the maximum absolute value of the $\eta\nu$ fermion (and $s\nu$ fermion) anti-binding energy per η-spinon pair (and spinon binding energy per spinon pair). It is given by $w_{\alpha\nu}^0 = W_{\alpha\nu}^h/\nu$ and can be expressed as follows,

$$
\begin{aligned}
w_{\alpha\nu}^0 &= \frac{1}{\nu}\,W_{\alpha\nu}^h = l_{\alpha\nu}^0\,W_{\alpha 1}^h\,; \quad l_{\alpha\nu}^0 \in [1/\nu, 1/\nu^2]\,, \\
l_{\alpha\nu}^0 &= 1/\nu\,, \quad u \to 0\,; \quad l_{\alpha\nu}^0 = 1/\nu^2\,, \quad u \to \infty\,.
\end{aligned}
\tag{177}
$$

Here $W_{s1}^h = 2\nu\mu_B\,|H|$ is the $s1$ band hole energy bandwidth provided in Eq. (166) and $W_{\eta 1}^h = W_{\eta 1}$. The latter energy scale reads $W_{\eta 1}^h = 2|\mu|$ for $u \to 0$ and vanishes in the limit $u \to \infty$, as given in Eq. (C23) of Appendix C.

The dependence on the number of pairs $\nu = 1, ..., \infty$ of the quantity $l_{\alpha\nu}^0$ of Eq. (177), which is the energy $w_{\alpha\nu}^0$ in units of $W_{\alpha 1}^h$, reveals that the maximum absolute value of the $\eta\nu$ fermion (and $s\nu$ fermion) anti-binding energy per η-spinon pair (and spinon binding energy per spinon pair) decreases for increasing pair number. Such an effect is stronger for larger values of u, with the ν dependence smoothly changing from $1/\nu$ for $u \ll 1$ to $1/\nu^2$ for $u \gg 1$.

H.   Transformation laws of the $\alpha\nu$ fermions under the electron - rotated-electron unitary transformation

Except for $u \to \infty$, the numbers of electron doubly occupied sites, electron unoccupied sites, spin-down electron singly occupied sites, and spin-up electron singly occupied sites are not good quantum numbers. As confirmed in Ref. [22], in general the expectation values of such numbers are u dependent. Only in the $u \to \infty$ limit do they equal the corresponding rotated-electron u-independent eigenvalues. The studies of that reference used objects in one-to-one correspondence to those of our description. In that reference such objects were directly associated with the BA quantum numbers and the spin and η-spin tower of states. (The relation of their operators to those of the original electrons was lacking and no relation to the representations of the model global $SO(3) \otimes SO(3) \otimes U(1)$ symmetry was established.)

Combination of the results of Ref. [22] with those of the present paper provides important information about the transformation laws of the $\alpha\nu$ fermions under the electron - rotated-electron unitary transformation. If one accounts for the different notations used here and in that reference, its results confirm that the deviations in the numbers of rotated-electron doubly occupied sites, rotated-electron unoccupied sites, spin-down rotated-electron singly occupied sites, and spin-up rotated-electron singly occupied sites due to creation or annihilation of c fermions, $\alpha\nu$ fermions, unbound η-spinons, and unbound spinons are u independent. They exactly equal the expected rotated-electron numbers eigenvalue deviations.

Furthermore, the results of Ref. [22] confirm that except for $u \to \infty$ the corresponding deviations in the expectations values of the numbers of electron doubly occupied sites, electron unoccupied sites, spin-up electron singly occupied sites, and spin-down electron singly occupied sites are a function of u. They are different from the deviations in the

corresponding rotated-electron numbers eigenvalues. That is consistent with for finite u values such electron numbers not being good quantum numbers.

There are two exceptions, though. As discussed in Section IV B, the first results from the $\pm 1/2$ unbound η-spinons and $\pm 1/2$ unbound spinons being invariant under the electron - rotated-electron unitary transformation. For the whole $u > 0$ range, creation onto a ground state of one $-1/2$ unbound η-spinon, one $+1/2$ unbound η-spinon, one $-1/2$ unbound spinon, and one $+1/2$ unbound spinon then exactly leads to a u-independent deviation in the expectation values of the corresponding electron occupancy numbers. Specifically, the deviations in the numbers of electron doubly occupied sites, electron unoccupied sites, spin-up electron singly occupied sites, and spin-down electron singly occupied sites, respectively, exactly equal one. This results from the unbound η-spinons and unbound spinons corresponding to the same η-spin and spin degrees of freedom occupancy configurations, respectively, in terms of electrons and rotated electrons.

There is a second exception. It refers to the $\alpha\nu$ fermions whose anti-binding energy ($\alpha = \eta$) or binding energy ($\alpha = s$), $\varepsilon^0_{\alpha\nu}(q)$, and velocity, $v_{\alpha\nu}(q) = \partial \varepsilon^0_{\alpha\nu}(q)/\partial q = \partial \varepsilon_{\alpha\nu}(q)/\partial q$, vanish. The requirement of $\alpha\nu$ fermion vanishing anti-binding or binding energy is fulfilled at limiting momentum values $q = \pm q_{\alpha\nu}$. At them the $\alpha\nu$ fermion dispersions are given by,

$$
\begin{aligned}
\varepsilon_{\eta\nu}(\pm q_{\eta\nu}) &= \nu\left[\varepsilon_{\eta,-1/2} + \varepsilon_{\eta,+1/2}\right] = (1 - \delta_{n,1})\, 2\nu|\mu| + \delta_{n,1}\, 2\nu\mu^0\,; \quad \varepsilon^0_{\eta\nu}(\pm q_{\eta\nu}) = 0\,, \\
\varepsilon_{s\nu}(\pm q_{s\nu}) &= \nu\left[\varepsilon_{s,-1/2} + \varepsilon_{s,+1/2}\right] = 2\nu\mu_B\,|H|\,; \quad \varepsilon^0_{s\nu}(\pm q_{s\nu}) = 0\,.
\end{aligned}
\tag{178}
$$

The results of Ref. [22] confirm that the $\alpha\nu$ fermions with limiting momentum values $q = \pm q_{\alpha\nu}$ are invariant under the electron - rotated-electron unitary transformation provided that their velocity vanishes,

$$
\begin{aligned}
v_{\alpha\nu}(q) &= \frac{\partial \varepsilon_{\alpha\nu}(q)}{\partial q}\Big|_{q = \pm q_{\alpha\nu}} = \frac{\partial \varepsilon^0_{\alpha\nu}(q)}{\partial q}\Big|_{q = \pm q_{\alpha\nu}} = 0\,, \\
\pm q_{\alpha\nu} &= \pm\frac{\pi}{L}\left(N_{a_{\alpha\nu}} - 1\right) = \pm\frac{\pi}{a_{\alpha\nu}}\left(1 - 1/N_{a_{\alpha\nu}}\right) \quad \text{for } N_{a_{\alpha\nu}} \text{ odd}\,, \\
\pm q_{\alpha\nu} &= \pm\frac{\pi}{L}\, N_{a_{\alpha\nu}} = \pm\frac{\pi}{a_{\alpha\nu}} \quad \text{for } N_{a_{\alpha\nu}} \text{ even}\,.
\end{aligned}
\tag{179}
$$

In general we use units of lattice constant a, so that $N_a = L$. On the other hand, here we have expressed the limiting momentum value of Eq. (117) in terms of the $\alpha\nu$ effective lattice spacing $a_{\alpha\nu}$, Eq. (136). This reveals that provided that $N_{a_{\alpha\nu}}/N_a \leq 1$ is finite and thus $N_{a_{\alpha\nu}} \gg 1$ for $N_a \gg 1$, the limiting momentum values $\pm q_{\alpha\nu}$ play the role of the Brillouin zone limits $\pm\pi/a_{\alpha\nu}$ of the $\alpha\nu$ momentum band.

The results of Ref. [22] confirm that for the whole $u > 0$ range creation onto a $n < 1$ (and $n > 1$) ground state of one $\eta\nu$ fermion fulfilling the above two requirements leads to a deviation in the expectation value of the number of electron doubly occupied (and unoccupied) sites that exactly equals the number of η-spinon pairs ν. Similarly, creation onto a $m > 0$ (and $m < 0$) ground state of one $s\nu$ fermion meeting the two above requirements leads for $u > 0$ to a deviation in the expectation value of the number of spin-down (and spin-up) electron singly occupied sites that again exactly equals the number of spinon pairs ν. In contrast, creation of one $\alpha\nu$ fermion that does not meet both requirements leads to u-dependent deviations in such electron-number expectation values.

The $\alpha\nu$ fermion vanishing velocity requirement is fulfilled at the limiting momentum values, $q = \pm q_{\alpha\nu}$, provided that the initial ground state has a vanishing $\alpha\nu$ fermion density, $N_{\alpha\nu}/N_a \to 0$, as $N_a \to \infty$. This requirement is met for $u > 0$ and arbitrary electronic density and spin density values by all $\alpha\nu$ branches other than the $s1$ branch. For the $s1$ branch it is met for $u > 0$ in the spin-density limits $m \to n$ for $n \in [0, 1]$ and $m \to (2 - n)$ for $n \in [1, 2]$. This follows from the $s1$ band ground-state occupancies being otherwise finite.

When the initial ground state has a vanishing $\alpha\nu$ fermion density and thus for finite u the $\alpha\nu$ fermion velocity vanishes at the limiting momentum values $q = \pm q_{\alpha\nu}$, its u dependence has a singular behavior at $u = 0$, becoming finite. Such $\alpha\nu$ fermion velocity behavior is confirmed by inspection of the slopes at the $\alpha\nu$ bands limiting momentum values of the $s1$, $s2$, $\eta1$, and $\eta2$ fermion energy dispersions plotted in Figs. 2, 3, 4, and 5.

An important consequence of the invariances considered here refers to particular case of one $s\nu \neq s1$ fermion (and $\eta\nu$ fermion) created onto a $S_s = 0$ (and $S_\eta = 0$) ground state. For instance, for an excited state with number values $N_{\alpha\nu} = 1$ and $N_{\alpha\nu'} = 0$ for $\nu' > \nu$ branches one confirms from the use of Eqs. (101) and (102) that $N_{a_{\alpha\nu}} = 1$. Thus the $\alpha\nu$ band consists of a single momentum, $q = \pm q_{\alpha\nu} = 0$. Furthermore, such an object energy reads $\varepsilon_{s\nu} = 0$ ($\alpha = s$) and $\varepsilon_{\eta\nu} = 2\nu\mu^0$ ($\alpha = \eta$), consistently with Eq. (178). In that single-momentum and single-energy state the $\alpha\nu$ fermion has vanishing velocity. Hence it is invariant under the electron - rotated-electron unitary transformation. The same applies to a finite number of $s\nu \neq s1$ fermions (and $\eta\nu$ fermions) created onto an initial $S_s = 0$ (and $S_\eta = 0$) ground state.

I.   The simplest excitations and the distinct types of elementary objects

The operator formulation considered in this paper accounts for the representations of the model global $SO(3) \otimes SO(3) \otimes U(1) = [SO(4) \otimes U(1)]/Z_2$ symmetry algebra. Here we discuss the relation of the simplest excitations to the representations of that symmetry algebra and the properties of the distinct types of elementary objects.

Consistent with the results of Appendix B, for a ground state with densities $n \in [0,1]$ and $m \in [0,n]$ the numbers of our formulation objects read,

$$\begin{aligned}
M_s &= M_s^{bo} + M_{s,+1/2}^{un} = N = n\,N_a\,; \quad M_s^{bo} = 2N_\downarrow\,; \quad M_{s,+1/2}^{un} = N_\uparrow - N_\downarrow = m\,N_a\,, \\
M_\eta &= M_\eta^{un} = M_{\eta,+1/2}^{un} = N_a - N = (1-n)\,N_a\,, \\
N_c &= N\,; \quad N_{s1} = N_\downarrow\,; \quad N_{s1}^h = N_\uparrow - N_\downarrow = m\,N_a\,.
\end{aligned} \tag{180}$$

Since the equality $N_c^h = [N_a - N_c]$ holds, here and below no values of N_c^h are given. For the present general ground state, the values of the following numbers vanish: $M_{\eta,-1/2}^{un}$, M_η^{bo}, $M_{s,-1/2}^{un}$, and set of all $\alpha\nu$ fermion numbers $\{N_{\alpha\nu}\}$ except that of the $s1$ fermions. For it the $s1$ band momenta are occupied for $q \in [-q_{Fs1}, q_{Fs1}] = [-k_{F\downarrow}, k_{F\downarrow}]$ and unoccupied for $|q| \in [q_{Fs1}, q_{s1}] = [k_{F\downarrow}, k_{F\uparrow}]$. The c band has the same occupancies as the $m = 0$ ground state whose object numbers are provided in Eq. (168).

1.   The elementary objects within spin excitations

Within the present representation the excitations associated with the N_{s1}^h $s1$ band holes refer to the spin degrees of freedom. However, alike the corresponding composite $s1$ fermions, the $s1$ fermion holes are spin-neutral objects. Consistent, in each unbound η-spinon and unbound spinon subspace, the $C_{N_{a_{s\nu}}}^{N_{s\nu}^h}$ configurations of the $N_{s\nu}^h$ $s\nu$ fermion holes are accounted for in the number $\mathcal{N}_{singlet}(S_s, M_s)$ of spin-singlet configurations, which is given in Eq. (125) for $\alpha = s$. Such spin-singlet configurations are different and independent from the $(2S_s + 1) = (M_s^{un} + 1)$ spin-multiplet configurations of the M_s^{un} unbound spin-1/2 spinons. Consistent with the expression given in Eq. (85), the spinon transformation laws under the electron - rotated-electron unitary transformation performed by the BA solution reveal that the spin S_s and spin projection $S_s^{x_3}$ values of an energy eigenstate are fully determined by the occupancies of such M_s^{un} unbound spinons.

Indeed, an important physical consequence of such transformation laws is the independence of the occupancy configurations of unbound spinons and bound spinons, respectively. The former and the latter are invariant and are not invariant under that transformation, respectively. One has found that the bound spinons exist within spin-neutral 2ν-spinon $s\nu$ fermions. Here $\nu = 1, ..., \infty$ is the number of spinons pairs. The latter objects live on an $s\nu$ effective lattice with a well-defined number, $N_{s\nu}$, of occupied sites ($s\nu$ fermions) and, $N_{s\nu}^h$, of unoccupied sites ($s\nu$ fermion holes). The conjugate coordinates of such sites spatial variables are the $s\nu$ band $N_{a_{s\nu}} = [N_{s\nu} + N_{s\nu}^h]$ discrete momentum values. A number $N_{s\nu}$ of those are occupied ($s\nu$ fermions) whereas $N_{s\nu}^h$ are unoccupied ($s\nu$ fermion holes). In units of $2\pi/N_a$, such discrete momentum values are the BA solution quantum numbers, Eq. (113).

The counting of the model global symmetry algebra representations of Section V B refers to *independent representations*. Their total number equals the Hilbert-space dimension 4^{N_a}, Eq. (124). Therefore, our above analysis of the $\mathcal{N}(S_s, M_s)$ spin configurations of each unbound η-spinon and unbound spinon subspace explicitly confirms that within the present representation the M_s^{un} unbound spin-1/2 spinons are different from the $N_{s\nu}^h$ $s\nu$ fermion holes. The unbound spin-1/2 spinons play the passive role of unoccupied sites of both the spin effective lattice and the corresponding $s\nu$ effective lattices. Thus the objects that move around in the spin effective lattice ring of length $L = N_{a_s}\,a_s = N_a\,a$ are the $s\nu$ fermions. In that motion they use all the $M_s^{un} = 2S_s$ unbound spinons and the $2(\nu' - \nu)$ bound spinons in the sets of $2(\nu' - \nu)$ sites of the spin effective lattice out of the $2\nu'$ sites occupied by each $s\nu'$ fermion with $2\nu' > 2\nu$ bound spinons. Note however that the holes in the corresponding BA $s\nu$ momentum bands exist in their own right and must not be treated as being the $M_s^{un} = 2S_s$ unbound spinons and $\sum_{\nu'=\nu+1}^{\infty} 2(\nu' - \nu)N_{s\nu'}$ unbound spinons that play the role of unoccupied sites. The $M_s^{un} = 2S_s$ unbound spinons have their independent occupancies and the $s\nu'$ fermion with $2\nu' > 2\nu$ bound spinons their own independent $s\nu'$ momentum bands. Consistent, the $s\nu$ effective lattice object motion can alternatively be described in terms of $s\nu$ fermions and $s\nu$ fermion holes, which in general have a finite velocity.

That the unbound spinons and $s\nu$ fermion holes are independent objects that describe different degrees of freedom of the spin $SU(2)$ symmetry algebra is confirmed by the studies of the second paper on the states spin currents. Consistent with the passive role played by the unbound spinons in the $s\nu$ fermion motion, such spin currents are found in that paper to be carried by the $s\nu$ fermion holes or $s\nu$ fermions. On the other hand, the effects on such

currents of the spin transverse fluctuations associated with spin-flipping the unbound spinons are fully controlled by such spin-1/2 objects, which exist on their own right.

Within the $N_a \rightarrow \infty$ limit, a $s\nu$ fermion moving around in the lattice ring of length $L = N_a\,a$ is exactly described by the same $s\nu$ fermion moving around in its $s\nu$ effective lattice ring of length $L = N_{a_{s\nu}}\,a_{s\nu} = N_a\,a$ and spacing $a_{s\nu} = L/N_{a_{s\nu}}$. Inspection of Eq. (102) reveals that such a $s\nu$ fermion does not "see" the spin-effective lattice sites occupied by $s\nu''$ fermions with a smaller number $\nu'' < \nu$ of spinon pairs. On the other hand, it uses the M_s^{un} sites of that effective lattice occupied by unbound spinons as $s\nu$ effective lattice unoccupied sites. Furthermore, it uses as well as $s\nu$ effective lattice unoccupied sites the $2(\nu' - \nu)$ sites of the former effective lattice out of the $2\nu'$ sites occupied by each $s\nu'$ fermion with $\nu' > \nu$ spinon pairs.

Within the present representation this does not imply however that M_s^{un} out of the $N_{s\nu}^h \geq M_s^{un}$ unoccupied sites of the $s\nu$ effective lattice should be identified with the M_s^{un} unbound spin-1/2 spinons. The remaining $[N_{s\nu}^h - M_s^{un}] \geq 0$ unoccupied sites of the $s\nu$ effective lattice neither should be identified with the sets of $2(\nu' - \nu)$ spin-1/2 spinons of each $s\nu'$ fermion of $\nu' > \nu$ branches with finite occupancy in the state. Those are also used by the $s\nu$ fermion as unoccupied sites of its $s\nu$ effective lattice.

For instance, let us consider an excited state of the ground state whose numbers are provided in Eq. (180). That excited has one four-spinon composite $s2$ fermion. Its spin degrees of freedom object numbers are,

$$
\begin{aligned}
M_s &= n\,N_a = [M_s^{un} + 2N_{s1} + 4N_{s2}]; \quad M_s^{un} = m\,N_a\,, \\
N_{s1} &= [(n-m)\,N_a/2 - 2]; \quad N_{s2} = 1\,, \\
N_{s1}^h &= [M_s^{un} + 2] = [m\,N_a + 2]; \quad N_{s2}^h = M_s^{un} = m\,N_a\,.
\end{aligned}
\tag{181}
$$

The excited-state $s2$ effective lattice has $N_{a_{s2}} = [N_{s2} + N_{s2}^h] = [m\,N_a + 1]$ sites. Hence the $s2$ fermion can move along its $s2$ effective lattice by interchanging position with each of the $M_s^{un} = m\,N_a$ sites occupied by unbound spinons in the underlying spin effective lattice. The $s2$ fermion does not "see" the $2N_{s1}$ spin-effective lattice sites occupied by the $s1$ fermions. On the other hand, the $N_{s1} = [(n-m)\,N_a/2 - 2]$ $s1$ fermions move along their $s1$ effective lattice by interchanging position with both each of the sites occupied by the $M_s^{un} = m\,N_a$ unbound spinons in the underlying spin effective lattice and two out of the four sites occupied by the spinons of the composite $s2$ fermion.

However, within the present representation neither M_s^{un} out of the $N_{s1}^h = [M_s^{un} + 2]$ $s1$ fermion holes nor the $N_{s2}^h = M_s^{un}$ $s2$ fermion holes should be identified with the M_s^{un} unbound spin-1/2 spinons. Those exist in their own right, their occupancies generating in this case $(2S_s + 1) = (M_s^{un} + 1) = (m\,N_a + 1)$ spin-multiplet configurations. Consistent, the occupancy configurations of the $N_{s1}^h = [M_s^{un}+2]$ $s1$ fermion holes and $N_{s2}^h = [M_s^{un}+2]$ $s2$ fermion holes generate different and independent $C_{N_{a_{s1}}}^{N_{s1}^h} = C_{n\,N_a}^{m\,N_a+2}$ and $C_{N_{a_{s2}}}^{N_{s2}^h} = C_{m\,N_a+1}^{m\,N_a} = m\,N_a + 1$ spin-singlet configurations, respectively. All such arguments apply as well to the spin-singlet excited states whose deviations are provided in Eq. (169), which are a particular case of the excited states under consideration.

Moreover, for an excited state whose generation from the general ground state with numbers provided in Eq. (180) breaks the spinon pair of one $s1$ fermion, giving rise to two unbound spinons, the spin degrees of freedom object numbers are,

$$
\begin{aligned}
M_s &= n\,N_a = [M_s^{un} + 2N_{s1}]; \quad M_s^{un} = [m\,N_a + 2]\,, \\
N_{s1} &= [(n-m)\,N_a/2 - 1]; \quad N_{s1}^h = M_s^{un} = [m\,N_a + 2]\,.
\end{aligned}
\tag{182}
$$

Here the values of the densities n and m are those of the initial ground state. The $N_{s1}^h = M_s^{un}$ $s1$ fermion holes of such an excited state should not be identified with the M_s^{un} unbound spin-1/2 spinons, yet their number exactly equals that of such objects. Those exist in their own right, their occupancies generating in this case $(M_s^{un} + 1) = (m\,N_a + 3)$ spin-multiplet configurations. On the other hand, the occupancy configurations of the $N_{s1}^h = M_s^{un}$ $s1$ fermion holes generate different and independent $C_{N_{a_{s1}}}^{N_{s1}^h} = C_{n\,N_a+1}^{m\,N_a+2}$ spin-singlet configurations. The same applies to the spin-triplet states whose deviations are given in Eq. (170), which are a particular case of the excited states considered here. In that case there are $(M_s^{un} + 1) = 3$ spin-triplet configurations. Each of these three configurations involve $M_s^{un} = 2$ spin 1/2 unbound spinons. Within our representation they are described by two unbound spinons with spin projection $+1/2$, one unbound spinon with spin projection $+1/2$ and one unbound spinon with spin projection $-1/2$, and two unbound spinons with spin projection $-1/2$, respectively.

2. *The elementary objects within excitations involving the three global symmetries*

Within the present representation $2S_c^h = [N_a - 2S_c]$ is the number of rotated-electron doubly occupied plus unoccupied sites. The independent occupancy configurations of the corresponding $M_\eta = [N_a - 2S_c]$ η-spin 1/2 η-spinons and

$N_c^h = [N_a - 2S_c]$ c fermion holes are associated with two degrees of freedom of the rotated-electron doubly-occupied sites and unoccupied sites occupancy configurations. Those refer to representations of the η-spin $SU(2)$ symmetry and c hidden $U(1)$ symmetry algebras, respectively.

As discussed in Section V B, a unbound η-spinon and unbound spinon subspace is spanned by all states with fixed values for the numbers S_η, $M_\eta = [N_a - 2S_c]$, and $N_c^h = [N_a - 2S_c]$. For each such a subspace the number of configurations of the $M_\eta = [N_a - 2S_c]$ η-spin-1/2 η-spinons is $\mathcal{N}(S_\eta, M_\eta)$, Eq. (121). On the other hand, the number of configurations of the $N_c^h = [N_a - 2S_c]$ of c fermion holes equals the dimension d_c, Eq. (103), which may be rewritten as $d_c = C_{N_a}^{N_c} = C_{N_a}^{N_c^h}$. The dimensions $\mathcal{N}(S_\eta, M_\eta)$ and d_c, which appear in the overall subspace dimension of Eq. (120), are found in Section V B to correspond to completely different and independent configurations. They refer to the number of subspace representations of the η-spin $SU(2)$ symmetry algebra and c hidden $U(1)$ symmetry algebra, respectively. The model global symmetry imposes that both the number $M_\eta = [N_a - 2S_c]$ of η-spin-1/2 η-spinons and $N_c^h = [N_a - 2S_c]$ of c fermion holes equal that $[N_a - 2S_c]$ of rotated-electron doubly plus unoccupied sites. Nonetheless within the present representation they are different and independent objects in their own right. Furthermore, consistent with the form of the number of subspace configurations $d_c = C_{N_a}^{N_c} = C_{N_a}^{N_c^h}$, the c fermions and c fermion holes alike are η-spin-less and spin-less objects.

We illustrate the issue discussed here in the case of the simplest one-electron addition excited states of the $\mu = 0$, $n = 1$, and $m = 0$ absolute ground state. The generation from it of such one-electron addition excited states involves changes in the degrees of freedom associated with the c hidden $U(1)$ symmetry and two $SU(2)$ symmetries. Under such an excitation, one $s1$ fermion spinon pair is broken. The created electron combines with one c fermion and that of the two spinons of the broken $s1$ fermion whose spin projection is opposite to its own. Such a process gives rise to one rotated-electron doubly occupied site. Its η-spin $SU(2)$ symmetry degrees of freedom are described by the $-1/2$ η-spinon created under the one-electron addition excitation. The c hidden $U(1)$ symmetry degrees of freedom account for the new rotated-electron doubly occupied site through the creation of one c fermion hole. Its available momentum values $q \in [-\pi, \pi]$ correspond to c band occupancy configurations that generate representations of the c hidden $U(1)$ symmetry algebra. They are associated with the dimension d_c in the excited subspace dimension given in Eq. (120). Such finite-velocity c fermion hole should not be identified with the $-1/2$ η-spinon also created under the transition to the excited state. There is also a spinon left behind by the $s1$ fermion spinon-pair breaking. It has the same spin projection as that of the created electron. Such a unpaired spinon becomes a unbound spinon in the excited state, which does not contribute to the state momentum. It should not be identified with the finite-velocity $s1$ fermion hole of momentum $q' \in [-\pi/2, \pi/2]$, which is also created as a result of the $s1$ fermion annihilation. Such unbound spinon and $s1$ fermion hole describe different spin degrees of freedom.

VI. QUANTUM PROBLEMS DESCRIBED BY THE 1D HUBBARD MODEL IN SUBSPACES OF PHYSICAL INTEREST

A. Symmetries and physically important subspaces

The combination of the present operator formulation with the PDT of Refs. [8–10] reveals that for the metallic phase of the 1D Hubbard model nearly the whole spectral weight associated with one- and two-electron excitations is generated by transitions from the ground state to both LHB excited states and first UHB excited states, as defined in Section V F. For electronic densities $n < 1$ and $n > 1$, the LHB (and first UHB) subspace is spanned by energy eigenstates with no (and one) rotated-electron doubly occupied site and unoccupied site, respectively.

The metallic-phase LHB subspace is a large subspace, which is spanned by 3^{N_a} energy eigenstates. Within it one has that $M_\eta^{bo} = 0$ so that the eigenvalue $2S_c$ of the c hidden $U(1)$ symmetry generator and the η-spin S_η are trivially related as $S_\eta = [N_a - 2S_c]/2$. For the 1D Hubbard model in that subspace the η-spin $SU(2)$ degrees of freedom play a minor role in charge and spin excitations that preserve the c fermion number $N_c = 2S_c$ and thus the η-spin S_η. Indeed, those of the energy eigenstates in that subspace that have the same η-spin value S_η have as well exactly the same η-spinon occupancy configuration. It refers to $M_\eta = M_{\eta,+1/2}^{un} = 2S_\eta$ (and $M_\eta = M_{\eta,-1/2}^{un} = 2S_\eta$) unbound η-spinons, all with the same η-spin projection.

Note however that excitations within that subspace as for instance one-electron addition and removal excitations under which the deviation $\delta M_\eta = \delta M_{\eta,-1/2}^{un} = 2\delta S_\eta$ is finite involve a change in such η-spin $SU(2)$ symmetry degrees of freedom occupancies. On the other hand, the charge and spin excitations within it conserve the c fermion and η-spinon numbers. Thus for them the quantum problem associated with the 1D Hubbard model in that subspace has effectively a charge $U(1)$ symmetry and a spin $SU(2)$ symmetry. Our results reveal that that charge $U(1)$ symmetry is the c hidden $U(1)$ symmetry, which is independent of the η-spin $SU(2)$ symmetry and η-spin $U(1)$ symmetry contained within it.

B. The quantum problem described by the 1D Hubbard model in the subspace with no rotated-electron doubly and unoccupied sites

Another important subspace is that spanned by half-filling energy eigenstates with both no rotated-electron doubly occupied sites and no rotated-electron unoccupied sites. The 1D Hubbard model in that subspace is the issue mainly addressed in this section. In it, that model becomes a spin-only problem. In the $u \gg 1$ limit it is the only finite-energy half-filling subspace. The relation within the $u \gg 1$ limit of the present representation spin-1/2 spinons to the excitations of the related 1D spin-1/2 isotropic Heisenberg antiferromagnetic model [26] is a problem briefly discussed in this section.

The subspace with no rotated-electron doubly-occupied and unoccupied sites contains the absolute ground state of vanishing chemical potential, $\mu = 0$, electronic density $n = 1$, and vanishing spin density $m = 0$. We call it *NDU subspace*, which stands for no (N) doubly-occupied (D) and no unoccupied (U) sites subspace. An energy scale that plays an important role in the energy spectrum of such a subspace is the minimum magnitude of the excitation energy $\Delta_{D_{rot}}$ for creation of a number $D_{rot} = M_\eta$ of rotated-electron doubly occupied sites and rotated-electron unoccupied sites onto a $n = 1$ and $m = 0$ ground state relative to its energy level. Such a ground-state energy level coincides with the zero-energy level of the Hamiltonian $\hat{H}$ of Eq. (1). Consistent with Eq. (88) and Eq. (175) for $n = 1$, it reads,

$$
\begin{aligned}
\min \Delta_{D_{rot}} &= \mu^0 M_\eta + \sum_{\sigma_\eta = \pm 1/2} (2\sigma_\eta) \mu M^{un}_{\eta,\sigma_\eta}, \quad \text{at} \ n = 1 \ \text{and} \ \mu \in [-\mu^0, \mu^0], \\
&= \mu^0 M_\eta, \quad \text{at} \ n = 1 \ \text{and} \ \mu = 0.
\end{aligned}
\tag{183}
$$

It follows from Eq. (183) that for one-electron and two-electron excited states the NDU subspace is for $u > 0$ the only Hilbert-space subspace for an excitation-energy window $\omega \in [0, \mu^0]$ and $\omega \in [0, 2\mu^0]$, respectively. Indeed within that excitation energy range there is neither rotated-electron doubly occupied sites nor rotated-electron unoccupied sites for the Hubbard model given in Eq. (2) at chemical potential $\mu = 0$. The energy eigenstates that span such a subspace are superpositions of a subset of local-rotated-electron states whose N_a sites are all singly occupied by rotated electrons. Moreover, the c fermion momentum band of such energy eigenstates is full.

The energy scale μ^0, which defines the excitation-energy range of the present quantum problem, is one half the Mott-Hubbard gap $2\mu^0$. Its exact u dependence is given in Eq. (C3) of Appendix C, whose $u \gg 1$ corresponding limiting behavior is $2\mu^0 \approx [U - 4t]$, as given in Eq. (C4) of that Appendix. Hence for $u \to \infty$ one has that $2\mu^0 \to \infty$, so that the NDU subspace is the only Hilbert-space subspace for all finite values of the excitation energy.

For such a subspace there is no η-spin effective lattice, whereas the spin effective lattice has N_a sites and is identical to the original lattice. The spin degrees of freedom of the $N = N_a$ rotated electrons that singly occupy the N_a sites are described by $M_{s,+1/2} = N_\uparrow$ spin-up and $M_{s,-1/2} = N_\downarrow = [N_a - N_\uparrow]$ spin-down spinons. The total number of spinons is thus fixed and given by $M_s = [M_{s,+1/2} + M_{s,-1/2}] = N_a = N$. The numbers M_s and $M_{s,\pm 1/2}$ can be written as the sum of two terms, which refer to unbound and bound spinons, respectively,

$$
M_s = N = M^{un}_s + M^{bo}_s = 2S_s + 2\sum_{\nu=1}^{\infty} \nu N_{s\nu},
$$

$$
M_{s,\pm 1/2} = M^{un}_{s,\pm 1/2} + M^{bo}_s/2 = [S_s \mp S^{x_3}_s] + \sum_{\nu=1}^{\infty} \nu N_{s\nu}.
\tag{184}
$$

Here $M^{un}_s = 2S_s$, $M^{un}_{s,\pm 1/2} = [S_s \mp S^{x_3}_s]$, and $M^{bo}_s = 2\sum_{\nu=1}^{\infty} \nu N_{s\nu}$.

Since there is no η-spin effective lattice and the c effective lattice is full, the important dimension is that given in Eq. (121) for $\alpha = s$,

$$
\begin{aligned}
\mathcal{N}(S_s, M_s) &= (2S_s + 1)\mathcal{N}_{singlet}(S_s, M_s) \\
&= (N - M^{bo}_s + 1)\mathcal{N}_{singlet}(N/2 - M^{bo}_s/2, N),
\end{aligned}
\tag{185}
$$

where

$$
\begin{aligned}
\mathcal{N}(S_s, M_s)_{singlet} &= C^{M_s/2 - S_s}_{M_s} - C^{M_s/2 - S_s - 1}_{M_s} \\
&= C^{M^{bo}_s/2}_N - C^{M^{bo}_s/2 - 1}_N,
\end{aligned}
\tag{186}
$$

and we used that $2S_s = [N - M^{bo}_s]$. The number of bound-spinon pairs $M^{bo}_s/2$ may have the values $M^{bo}_s/2 = 0, 1, 2, ..., N/2$, so that the Hilbert-space dimension of the quantum problem corresponding to the half-filled 1D Hub-

bard model in the NDU subspace is,

$$d_{ndu} = \sum_{M_s^{bo}/2=0}^{N/2} (N - M_s^{bo} + 1) \left\{ C_N^{M_s^{bo}/2} - C_N^{M_s^{bo}/2-1} \right\} = 2^N = 2^{N_a} . \tag{187}$$

Since in that subspace there is only rotated-electron single occupancy, upon acting onto it, the ηs local quasi-spin operators of Eq. (66) simplify to,

$$\tilde{q}_j^- = \tilde{s}_{j,s}^- = \tilde{c}_{j,\uparrow}^\dagger \tilde{c}_{j,\downarrow}; \quad \tilde{q}_j^+ = \tilde{s}_{j,s}^+ = (\tilde{s}_{j,s}^-)^\dagger; \quad \tilde{q}_j^{x_3} = \tilde{s}_{j,s}^{x_3} = -(\tilde{n}_{j,\uparrow} - \tilde{n}_{j,\downarrow})/2 . \tag{188}$$

Furthermore, again accounting for the lack of both rotated-electron doubly occupied sites and unoccupied sites, upon writing the Hamiltonian of Eq. (73) in the NDU subspace, one finds that all its terms of odd order vanish and the terms of even order simplify to,

$$\begin{aligned}
\hat{H}^{(0)} &= U \tilde{V}^c , \\
\hat{H}^{(2)} &= -\frac{t^2}{U} \tilde{T}_{-1} \tilde{T}_{+1} , \\
\hat{H}^{(4)} &= \frac{t^4}{U^3} [\tilde{T}_{-1} \tilde{T}_{+1} \tilde{T}_{-1} \tilde{T}_{+1} - \frac{1}{2} \tilde{T}_{-1}^2 \tilde{T}_{+1}^2 - \tilde{T}_{-1} \tilde{T}_0^2 \tilde{T}_{+1}] .
\end{aligned} \tag{189}$$

Within the NDU subspace, the contributing Hamiltonian terms of Eq. (189) belonging to the general term $\tilde{T}_{-1}^2 \tilde{T}_{+1}^2$ are of the form $\tilde{T}_{-1;j,j'} \tilde{T}_{+1;j,j'} \tilde{T}_{-1;j'',j'''} \tilde{T}_{+1;j'',j'''}$ where both nearest-neighboring sites of indices j and j' are different from the two nearest-neighboring sites of indices j'' and j'''. Moreover, in the Hamiltonian term containing $\tilde{T}_{-1} \tilde{T}_0^2 \tilde{T}_{+1}$, the contributing terms are of the forms $\tilde{T}_{-1;j,j'} \tilde{T}_{0;j,j''} \tilde{T}_{0;j,j''} \tilde{T}_{+1;j'',j'''} \tilde{T}_{+1;j,j'}$ or $\tilde{T}_{-1;j,j'} \tilde{T}_{0;j',j'''} \tilde{T}_{0;j',j'''} \tilde{T}_{+1;j'',j'''} \tilde{T}_{+1;j,j'}$ where $j'' \neq j'$ and $j''' \neq j$, respectively. In addition, after some straightforward algebra one finds that within the NDU subspace all products of operators $F_{\gamma;j,j'}$ of Eq. (71) in the corresponding products of rotated kinetic operators $\tilde{T}_\gamma = -[t/U] \sum_{\langle j,j' \rangle} F_{\gamma;j,j'} \tilde{Q}_{|\gamma|;j,j'}$ of Eq. (70) appearing in the Hamiltonian terms provided in Eq. (189) can be expressed only in terms of local operators $\tilde{q}_j^c$ and $\tilde{q}_{j'}^c$. In the NDU subspace one can then replace such operators by their eigenvalue, which is 1. Thus the Hamiltonian terms of Eq. (189) can be expressed in terms of only spinon operators. Moreover, the zeroth-order term becomes a mere constant, $\hat{H}^{(0)} = [U/4] N_a$, and may be ignored.

In addition, by manipulations of the commutators of Eq. (72), we find that for the Hamiltonian in the NDU subspace the term of sixth order can also be expressed only in terms of spinon operators. In the present 1D case the problem simplifies, since many contributions vanish, and one expresses the commutators of Eq. (72) directly in terms such operators. Fortunately, at $n = 1$ there is no need of deriving the Hamiltonian sixth order term expression explicitly in terms of the three rotated kinetic operators, in contrast to for densities $n \neq 1$. That is a more involved problem that we do not address here.

In order to make our notation compact, we use in the following Hamiltonian expression the spinon operator vector $\vec{\tilde{s}}_{j,s}$ whose operator components are $\tilde{s}_{j,s}^{x_1}$, $\tilde{s}_{j,s}^{x_2}$, and $\tilde{s}_{j,s}^{x_3}$. Upon expressing the Hamiltonian operators $\hat{H}^{(2)}$ and $\hat{H}^{(4)}$ of Eq. (189) along with the Hamiltonian operator $\hat{H}^{(6)}$ in terms of spinon operators we find after some algebra,

$$\begin{aligned}
\hat{H}_{symm} &= \hat{H}^{(2)} + \hat{H}^{(4)} + \hat{H}^{(6)} + ... , \\
\hat{H}^{(2)} &= -\frac{t^2}{U} \sum_{j=1}^{N_a} (1 - 4 \vec{\tilde{s}}_{j,s} \cdot \vec{\tilde{s}}_{j+1,s}) , \\
\hat{H}^{(4)} &= -\frac{t^4}{U^3} \sum_{j=1}^{N_a} \left[-4(1 - 4 \vec{\tilde{s}}_{j,s} \cdot \vec{\tilde{s}}_{j+1,s}) + (1 - 4 \vec{\tilde{s}}_{j,s} \cdot \vec{\tilde{s}}_{j+2,s}) \right] , \\
\hat{H}^{(6)} &= -\frac{t^6}{U^5} \sum_{j=1}^{N_a} 2 \left[15(1 - 4 \vec{\tilde{s}}_{j,s} \cdot \vec{\tilde{s}}_{j+1,s}) - 6(1 - 4 \vec{\tilde{s}}_{j,s} \cdot \vec{\tilde{s}}_{j+2,s}) + (1 - 4 \vec{\tilde{s}}_{j,s} \cdot \vec{\tilde{s}}_{j+3,s}) \right] \\
&\quad + \frac{t^6}{U^5} \sum_{j=1}^{N_a} \left[(1 - 4 \vec{\tilde{s}}_{j,s} \cdot \vec{\tilde{s}}_{j+3,s})(1 - 4 \vec{\tilde{s}}_{j,s} \cdot \vec{\tilde{s}}_{j+2,s}) - (1 - 4 \vec{\tilde{s}}_{j,s} \cdot \vec{\tilde{s}}_{j+2,s})(1 - 4 \vec{\tilde{s}}_{j,s} \cdot \vec{\tilde{s}}_{j+3,s}) \right] . \tag{190}
\end{aligned}$$

For the corresponding spin excited states, such expressions are valid at $\mu = 0$ and excitation energy $\omega < 2\mu^0$. Note that in the NDU subspace the expression of the Hamiltonian operators $\hat{H}^{(4)}$ and $\hat{H}^{(6)}$ do not include terms multiplying

the non-universaly valued real-number parameter θ. Therefore, their expressiona are fully known and given in Eq. (190).

The $\mu = 0$, $n = 1$, $m = 0$ absolute ground-state energy is to t^6/U^5 order readily obtained from the general ground-state energy expansion derived in Ref. [55] for $n \in [0,1]$ and $m = 0$. By choosing $n = 1$ in that general expansion we find,

$$E_{GS}^0/N_a = -\frac{t^2}{U} 4 \ln 2 + \frac{t^4}{U^3} 9 \zeta(3) - \frac{t^6}{U^5} 75 \zeta(5) + ... , \tag{191}$$

where $\zeta(3)$ and $\zeta(5)$ are Riemann Zeta functions. This ground-state energy refers to the Hamiltonian expression to t^6/U^5 order given in Eq. (190).

VII.   THE 1D HUBBARD MODEL IN THE NDU SUBSPACE FOR $u \gg 1$

For $u \gg 1$ the leading-order term $\hat{H}^{(2)}$ of the Hamiltonian expression provided in Eq. (190) becomes dominant, so that in the NDU subspace that Hamiltonian approximately reads,

$$\hat{H}_{symm} \approx -\frac{4\,t^2}{U} \sum_{j=1}^{N} \left(\frac{1}{4} - \vec{\hat{s}}_{j,s} \cdot \vec{\hat{s}}_{j+1,s} \right) , \tag{192}$$

where $N = N_a$. Within the $u \gg 1$ limit the rotated electrons become electrons, so that the local spinon operators $\vec{\hat{s}}_{j,s}$ defined in Eqs. (64) and (67) that appear in Eq. (190) were here replaced by the corresponding unrotated local spin operators, $\vec{\hat{s}}_{j,s}$, provided in Eq. (42). Consistent with the known $u \gg 1$ relation of the half-filled 1D Hubbard model to the 1D isotropic Heisenberg antiferromagnetic model of spins 1/2, for exchange constant $J = 4\,t^2/U$ the expression given in Eq. (192) is exactly that of the latter model.

Since in the $u \gg 1$ limit the N rotated electrons become the N electrons, the $M_s = N$ spin-1/2 spinons of the present formulation become the spins of each of the N electrons. At $N = N_a$ the NDU subspace becomes the only finite-energy subspace as $u \to \infty$. Within it the spin and charge degrees of freedom are decoupled, so that the spins of each of the half-filled 1D Hubbard model N electrons become the N spins of the 1D spin-1/2 isotropic Heisenberg antiferromagnetic model. Thus at half filling and for $u \to \infty$ the $M_s = N$ spin-1/2 spinons of the present formulation become such N spin-1/2 spins.

This reveals that in such a limit the spin-1/2 spinons of the present electron and rotated-electron vacuum normal-ordered formulation and the spin-1/2 spin waves of the ground-state normal-ordered description of Ref. [26] are completely distinct quantum objects. Indeed, the $S_\eta = 0; S_s = 0; 2S_c = N_a$ absolute ground state of the 1D Hubbard model is populated by $N = N_a$ spin-1/2 spinons, as defined in the present formulation, whereas it contains no spin-1/2 spinons, as defined in Refs. [29, 30]. Alike the spin-1/2 spin waves of Ref. [26] are excitations of the zero-spin ground state of the 1D isotropic Heisenberg antiferromagnetic model, the spin-1/2 spinons of Refs. [29, 30] have been constructed inherently to be excitations of the $S_\eta = 0; S_s = 0; 2S_c = N_a$ absolute ground state of the 1D Hubbard model.

The relation for $u \gg 1$ of the N spin-1/2 spinons of the present formulation to the spin-1/2 spin waves of Ref. [26] is in terms of electrons exactly the same as that for $u > 0$ of the spin-1/2 spinons of the present formulation to the spin-1/2 spinons of Refs. [29, 30] in terms of rotated electrons. Thus we forward the reader to the second paper, Ref. [18], for further information on the relation between the present spin-1/2 spinons and those of the ground-state normal-ordered traditional spinon descriptions.

Importantly, in the second paper it is confirmed that there is no contradiction whatsoever between the spin-1/2 spinons of the present formulation and those of Refs. [28–30]. The former and the latter spinon definitions are normal ordered relative to the electron and rotated-electron vacuum and an initial $S_s = 0$ ground state, respectively. The two types of spin-1/2 spinons are confirmed to be distinct elementary objects associated with uniquely related scattering-state basis choices. The possibility of such different choices stems from the degeneracy of the excited energy eigenstates of the $S_s = 0$ ground state with the same number of spin-1/2 spinons as defined in Refs. [28–30].

VIII.   CONCLUDING REMARKS

Since the BA solution of the 1D Hubbard model is exact, most results of studies by means of that solution are correct independently of the interpretation of which elementary objects are involved in its excitations. However, the relation of the operators of the elementary objects to those of the original electrons is an issue of highest importance

for the physical interpretation of such results. Unfortunately, the unique definition of the elementary objects operators and their relation to the electron creation and annihilated operators remains for most object representations an open problem. That unsolved problem is one of the main motivations of this paper. Indeed, the charge-spin separation and corresponding interpretations in terms of exotic objects such as holons and spinons play a major role in the interpretation and description of the low-dimensional correlated systems physics.

The operator formulation introduced in this paper goes beyond the BA solution subspace. It has been constructed inherently to spinon, η-spinon, and c fermion occupancy configurations generating *all* 4^{N_a} energy eigenstates. Concerning the general problem of the 1D Hubbard model in its full Hilbert space, our results confirm that there occurs a three degrees of freedom separation associated with the two previously known spin $SU(2)$ and η-spin $SU(2)$ symmetries plus the c hidden $U(1)$ symmetry found in Ref. [19]. From such three symmetries three types of elementary objects follow: The spin-1/2 spinons, the η-spin-1/2 η-spinons, and the spin-less and η-spin-less c fermions, respectively. The corresponding c fermion operators and ηs quasi-spin operators whose expressions are provided in Eqs. (61) and (67), respectively, are mapped from the rotated-electron operators by an exact local transformation that does not introduce constraints. The same applies to the related spinon and η-spinon operators defined in terms of the local c fermion number operators and ηs quasi-spin operators in Eq. (66). On the other hand, the electron - rotated-electron unitary operator is defined in Section II B it terms of its $4^{N_a} \times 4^{N_a}$ matrix elements given in Eqs. (51) and (52). Profiting from the interplay of the exact BA solution with the model global symmetry algebra representations, we have found which of these matrix elements vanish. Those that are finite have been expressed in terms of exact BA amplitudes, which we have extended to the non-LWSs generated from the Bethe states.

The transformation laws under the electron - rotated-electron unitary transformation of the $M_s = N_R^s = 2S_c$ spinons (and $M_\eta = N_R^\eta = [N_a - 2S_c]$ η-spinons) imply that $M_s^{bo} = [2S_c - 2S_s]$ of such spinons (and $M_\eta^{bo} = [N_a - 2S_c - 2S_\eta]$ of such η-spinons) are bound (and anti-bound) within spin-neutral (and η-spin-neutral) composite $s\nu$ fermions (and $\eta\nu$ fermions). Although the physical meaning of the eigenvalue $2S_c$ of the c hidden $U(1)$ symmetry and of the numbers M_s^{bo} and M_η^{bo} remained masked by the underlying mathematical formalism, we have shown that they appear in the exact BA thermodynamic equations introduced in Ref. [1]. As confirmed in this paper, that solution explicitly accounts for the model global symmetry and corresponding transformation laws under the electron - rotated-electron unitary transformation. This is for instance explicit in the form that the rotated-electron amplitudes given in Eqs. (53) and (54) have for all 4^{N_a} energy eigenstates.

The model global $[SO(4) \otimes U(1)]/Z_2 = SO(3) \otimes SO(3) \otimes U(1)$ symmetry accounted for by the operator formulation introduced in this paper applies as well to the Hubbard model on any bipartite lattice. The studies of Ref. [56] present an approximate operator formulation to the model on the square lattice. Its motivation and starting point is that introduced here for the 1D Hubbard model, in terms of quantities extracted from the exact BA solution.

Several properties predicted by the 1D Hubbard model were observed in low-dimensional complex materials [5, 57]. The investigations presented in Refs. [11, 58] confirm that the PDT successfully describes the unusual finite-energy spectral features observed by angle-resolved photoelectron spectroscopy in quasi-1D organic metals. The results presented here and in the ensuing paper contribute to the further understanding of the microscopic non-perturbative mechanisms behind these properties. In the second paper it is shown that the scatterers and scattering centers that naturally emerge from the present elementary-objects operator formulation for the 1D Hubbard model are the spin-less and η-spin-less c pseudofermions, the spin-neutral composite $s\nu$ pseudofermions, and the η-spin-neutral composite $\eta\nu$ pseudofermions. Those are related to the c fermions, $s\nu$ fermions, and $\eta\nu$ fermions, respectively, by a unitary transformation. For the excited states, it slightly shifts the discrete momentum values of such objects. Otherwise the c fermions, $s\nu$ fermions, and $\eta\nu$ fermions that emerge from our rotated-electron operator formulation and the corresponding c pseudofermions, $s\nu$ pseudofermions, and $\eta\nu$ pseudofermions, respectively, studied in the second paper have the same properties.

The pseudofermion scattering theory and corresponding dressed S matrices and phase shifts are shown in the second paper to control the spectral-weight distributions of the PDT [8–10]. Specifically, such dressed S matrices control the momentum, electronic density, spin density, and repulsive interaction dependence of the spectral-function exponents associated with the high-energy behavior beyond the linear Luttinger-theory predictions revealed by the PDT for the 1D Hubbard model and more recently by the methods of Refs. [12–14, 17] for a wider class of integrable and non-integrable 1D correlated problems. The relation of the present formulation elementary objects to traditional spinon and holon descriptions as those of Refs. [28–30] is an issue that is also investigated in the second paper, Ref. [18]. As mentioned in previous sections, it is found in that paper that there is no contradiction whatsoever between such distinct elementary objects choices and corresponding scattering theories. The possibility of different choices of both elementary objects and scattering states is found to stem from the degeneracy of the excited energy eigenstates that span the subspaces of the corresponding scattering theories.

Acknowledgments

Appendix A: Useful quantities and transformations

In this Appendix we introduce the known model L-matrix expression. Furthermore, it is confirmed that the operational expressions of the rotated-electron operators in terms of ηs quasi-spin operators and c fermion operators, Eq. (69), give the correct results upon their application onto the one-site states $|j, \odot, h_c\rangle$, $|j, \uparrow\downarrow, h_c\rangle$, $|j, \uparrow, p_c\rangle$, and $|j, \downarrow, p_c\rangle$ appearing on the right-hand side of Eq. (82).

The known expression in terms of electron creation and annihilation operators of the BA inverse-scattering method on-site 4×4 L-matrix $\mathcal{L}_j(\lambda)$ of Eq. (60) is [43],

$$\mathcal{L}_j = \begin{bmatrix} -e^h\, g_{j,\uparrow}\, g_{j,\downarrow} & -g_{j,\uparrow}\, c_{j,\downarrow} & i\, c_{j,\uparrow}\, g_{j,\downarrow} & i\, c_{j,\uparrow}\, c_{j,\downarrow}\, e^h \\ -i\, g_{j,\uparrow}\, c_{j,\downarrow}^\dagger & e^{-h}\, g_{j,\uparrow}\, g_{j,\downarrow}^h & e^{-h}\, c_{j,\uparrow}\, c_{j,\downarrow}^\dagger & i\, c_{j,\uparrow}\, g_{j,\downarrow}^h \\ c_{j,\uparrow}^\dagger\, f_{j,\downarrow} & e^{-h}\, c_{j,\uparrow}^\dagger\, c_{j,\downarrow} & e^{-h}\, g_{j,\uparrow}^h\, g_{j,\downarrow} & i\, g_{j,\uparrow}^h\, c_{j,\downarrow} \\ -i\, e^h\, c_{j,\uparrow}^\dagger\, c_{j,\downarrow}^\dagger & c_{j,\uparrow}^\dagger\, g_{j,\downarrow}^h & i\, g_{j,\uparrow}^h\, c_{j,\downarrow}^\dagger & -i\, g_{j,\uparrow}^h\, g_{j,\downarrow}^h\, e^h \end{bmatrix} \tag{A1}$$

where

$$g_{j,\sigma} = i\,[a\, n_{j,\sigma} - ib\, n_{j,\sigma}^h]\,; \quad g_{j,\sigma}^h = [a\, n_{j,\sigma}^h - ib\, n_{j,\sigma}]\,, \tag{A2}$$

and $n_{j,\sigma}^h = (1 - n_{j,\sigma})$. It is shown in this paper that it can be expressed in terms of the seven generators of the local gauge $SU(2) \otimes SU(2) \otimes U(1)$ symmetry of the 1D Hubbard model at $t = 0$ and corresponding spin-less and η-spin-less fermion operators, as given in Eq. (60).

The seven local operators obtained by electron rotation of such generators are expressed in Eq. (67) in terms of the ηs quasi-spin operators and c fermion operators defined in this paper. Application of the operational expressions of the rotated-electron operators in terms of such ηs quasi-spin operators and c fermion operators provided in Eq. (69) onto the one-site states $|j, \odot, h_c\rangle$, $|j, \uparrow\downarrow, h_c\rangle$, $|j, \uparrow, p_c\rangle$, and $|j, \downarrow, p_c\rangle$ leads to,

$$\begin{aligned} \tilde{c}_{j,\uparrow}^\dagger |j, \uparrow, p_c\rangle &= (-1)^j\, f_{j,c} \left(\frac{1}{2} + \tilde{q}_j^{x_3} \right) |j, \uparrow, p_c\rangle = 0\,, \\ \tilde{c}_{j,\uparrow}^\dagger |j, \downarrow, p_c\rangle &= (-1)^j\, f_{j,c} \left(\frac{1}{2} + \tilde{q}_j^{x_3} \right) |j, \downarrow, p_c\rangle = (-1)^j\, f_{j,c} |j, \downarrow, p_c\rangle = |j, \uparrow\downarrow, h_c\rangle\,, \\ \tilde{c}_{j,\uparrow}^\dagger |j, \odot, h_c\rangle &= f_{j,c}^\dagger \left(\frac{1}{2} - \tilde{q}_j^{x_3} \right) |j, \odot, h_c\rangle = f_{j,c}^\dagger |j, \odot, h_c\rangle = |j, \uparrow, p_c\rangle\,, \\ \tilde{c}_{j,\circ}^\dagger |j, \uparrow\downarrow, h_c\rangle &= f_{j,c}^\dagger \left(\frac{1}{2} - \tilde{q}_j^{x_3} \right) |j, \uparrow\downarrow, h_c\rangle = 0\,, \end{aligned} \tag{A3}$$

and

$$\begin{aligned} \tilde{c}_{j,\downarrow}^\dagger |j, \uparrow, p_c\rangle &= (-1)^j\, f_{j,c}\, \tilde{q}_j^+ |j, \uparrow, p_c\rangle = (-1)^j\, f_{j,c} |j, \downarrow, p_c\rangle = |j, \uparrow\downarrow, h_c\rangle\,, \\ \tilde{c}_{j,\downarrow}^\dagger |j, \downarrow, p_c\rangle &= (-1)^j\, f_{j,c}\, \tilde{q}_j^+ |j, \downarrow, p_c\rangle = 0\,, \\ \tilde{c}_{j,\downarrow}^\dagger |j, \odot, h_c\rangle &= f_{j,c}^\dagger\, \tilde{q}_j^+ |j, \odot, h_c\rangle = (-1)^j\, f_{j,c}^\dagger |j, \uparrow\downarrow, h_c\rangle = |j, \downarrow, p_c\rangle\,, \\ \tilde{c}_{j,\downarrow}^\dagger |j, \uparrow\downarrow, h_c\rangle &= f_{j,c}^\dagger\, \tilde{q}_j^+ |j, \uparrow\downarrow, h_c\rangle = 0\,. \end{aligned} \tag{A4}$$

Hence for the rotated-electron annihilation operators the result is,

$$
\begin{aligned}
\tilde{c}_{j,\uparrow}|j,\sigma,c\rangle &= f_{j,c}\left(\frac{1}{2}-\tilde{q}_j^{x_3}\right)|j,\uparrow,p_c\rangle = f_{j,c}|j,\uparrow,p_c\rangle = |j,\odot,h_c\rangle\,, \\
\tilde{c}_{j,\uparrow}|j,\downarrow,p_c\rangle &= f_{j,c}\left(\frac{1}{2}-\tilde{q}_j^{x_3}\right)|j,\downarrow,p_c\rangle = 0\,, \\
\tilde{c}_{j,\uparrow}|j,\odot,h_c\rangle &= (-1)^j f_{j,c}^\dagger\left(\frac{1}{2}+\tilde{q}_j^{x_3}\right)|j,\odot,h_c\rangle = 0\,, \\
\tilde{c}_{j,\uparrow}|j,\uparrow\downarrow,h_c\rangle &= (-1)^j f_{j,c}^\dagger\left(\frac{1}{2}+\tilde{q}_j^{x_3}\right)|j,\uparrow\downarrow,h_c\rangle = (-1)^j f_{j,c}^\dagger|j,\uparrow\downarrow,h_c\rangle = |j,\downarrow,p_c\rangle\,,
\end{aligned}
\tag{A5}
$$

and

$$
\begin{aligned}
\tilde{c}_{j,\downarrow}|j,\uparrow,p_c\rangle &= f_{j,c}\,\tilde{q}_j^-\,|j,\uparrow,p_c\rangle = 0\,, \\
\tilde{c}_{j,\downarrow}|j,\downarrow,p_c\rangle &= f_{j,c}\,\tilde{q}_j^-\,|j,\downarrow,p_c\rangle = f_{j,c}|j,\uparrow,p_c\rangle = |j,\odot,h_c\rangle\,, \\
\tilde{c}_{j,\downarrow}|j,\odot,h_c\rangle &= (-1)^j f_{j,c}^\dagger\,\tilde{q}_j^-\,|j,\odot,h_c\rangle = 0\,, \\
\tilde{c}_{j,\downarrow}|j,\uparrow\downarrow,h_c\rangle &= (-1)^j f_{j,c}^\dagger\,\tilde{q}_j^-\,|j,\uparrow\downarrow,h_c\rangle = f_{j,c}^\dagger|j,\odot,h_c\rangle = |j,\uparrow,p_c\rangle\,.
\end{aligned}
\tag{A6}
$$

In the above equations it was used that, as given in Eq. (67), the operator $\tilde{q}_j^l$ where $l = x_3,\pm$ reads $\tilde{q}_j^l = \tilde{s}_{j,s}^l$ (and $\tilde{q}_j^l = \tilde{s}_{j,\eta}^l$) when the site j is singly occupied by rotated electrons (and unoccupied or doubly occupied by rotated electrons.)

Analysis of Eqs. (A3)-(A6) confirms that the correct final states are obtained.

Appendix B: Unbound spinon and unbound η-spinon energies and ground-state occupancies

In this Appendix the energies of the $\pm 1/2$ unbound η-spinons are explicitly derived. A similar analysis provides those of the $\pm 1/2$ unbound spinons. The BA solution subspace is smaller than and contained in the 1D Hubbard model full Hilbert space. Thus analysis of the energy spectra of the Bethe states alone is not enough to clarify the problem of the ground-state occupancies. Here we combine the model global symmetry with the BA solution to also address that problem.

For simplicity, to start with we consider $m = 0$ ground states of the Hamiltonian of Eq. (1) at zero magnetic field,

$$
\hat{H} = \hat{H}_{symm} - \mu\,2\hat{S}_\alpha^{x_3} = \hat{H}_{symm} - \mu\,(\hat{N} - N_a)\,,
\tag{B1}
$$

where $\hat{H}_{symm}$ is given in Eq. (2).

For $u > 0$ we denote by E_{GS}^0 and E_{GS} the ground-state energy eigenvalues of the Hamiltonians $\hat{H}_{symm}$ and $\hat{H}$ given in Eqs. (2) and (B1), respectively,

$$
\begin{aligned}
E_{GS}^0(S_\eta) &= \langle GS|\hat{H}_{symm}|GS\rangle\,, \\
E_{GS}(S_\eta, S_\eta^{x_3}) &= \langle GS|\hat{H}|GS\rangle = E_{GS}^0(S_\eta) - \mu\,(N - N_a) = E_{GS}^0(S_\eta) + \mu\,x\,N_a\,.
\end{aligned}
\tag{B2}
$$

Here $x = (1 - n)$ denotes the hole concentration.

The Hamiltonian provided in Eq. (B1) describes the same quantum problem as the Hamiltonian $\hat{H}_{symm}$, Eq. (2), but refers to the grand-canonical ensemble. Since the latter Hamiltonian commutes with $-\mu\,2\hat{S}_\alpha^{x_3}$, one has that the two Hamiltonians commute, $[\hat{H}_{symm}, \hat{H}] = 0$. Thus they have the same energy eigenstates. Only the corresponding energy eigenvalues are in general different. Those of $\hat{H}$ are shifted relative to the energy eigenvalues of $\hat{H}_{symm}$ by $-\mu\,(N - N_a) = \mu\,x\,N_a$. Hence the following relation holds for all 4^{N_a} energy eigenstates $|\Psi_{l_o,l_\triangle,u}\rangle$,

$$
\begin{aligned}
\langle\Psi_{l_o,l_\triangle,u}|\hat{H}|\Psi_{l_o,l_\triangle,u}\rangle &= \langle\Psi_{l_o,l_\triangle,u}|\hat{H}_{symm}|\Psi_{l_o,l_\triangle,u}\rangle - \mu\,(N - N_a) \\
&= \langle\Psi_{l_o,l_\triangle,u}|\hat{H}_{symm}|\Psi_{l_o,l_\triangle,u}\rangle + \mu\,x\,N_a\,.
\end{aligned}
\tag{B3}
$$

We start by assuming that for electronic densities $n < 1$ (and $n > 1$) the ground state is a LWS (and HWS) of the η-spin symmetry algebra. We then use symmetry arguments to confirm that this is so. The zero-energy level of the

Hamiltonian $\hat{H}$, Eq. (B1), corresponds to the initial ground-state energy. For that Hamiltonian the set of $2S_\eta$ tower energy eigenstates generated by application onto the $n < 1$ ground state of the off-diagonal generator of the η-spin algebra $\hat{S}^\dagger_\eta$ a number of times $n_\eta = 1, ..., 2S_\eta$ have energy eingenvalue $\langle \Psi_{l_o,l_\triangle,u}|\hat{H}_{symm}|\Psi_{l_o,l_\triangle,u}\rangle + 2n_\eta|\mu|$. Thus out of the corresponding tower of $2S_\eta + 1$ energy eigenstates, that corresponding to $n_\eta = 0$ has lowest energy.

However, to confirm that for $n < 1$ the ground state is a η-spin algebra LWS we must consider a $n < 1$ ground state other than that belonging to the η-spin tower. Specifically, $n < 1$ ground states with the same electron numbers as the tower states of energy $\langle \Psi_{l_o,l_\triangle,u}|\hat{H}_{symm}|\Psi_{l_o,l_\triangle,u}\rangle + 2n_\eta|\mu|$. Hence, out of the such tower states, only those having electronic densities $n < 1$ and thus $n_\eta < S_\eta$ are of interest. The $n < 1$ ground states under consideration have η spin and η-spin projection $(S_\eta - \delta S_\eta)$ and $-(S_\eta - \delta S_\eta)$, respectively, where $\delta S_\eta = n_\eta$. Here S_η is the η-spin value of the LWSs of the η-spin tower and $n_\eta < S_\eta$. Provided that the inequality $0 < \delta S_\eta < S_\eta$ holds, one has in the thermodynamic limit that the two ground-state energy eigenvalues under consideration of the Hamiltonian $\hat{H}$ of Eq. (B1) are such that,

$$E_{GS}(S_\eta, -S_\eta) = E_{GS}(S_\eta - \delta S_\eta, -S_\eta + \delta S_\eta).\tag{B4}$$

This relation follows from in the thermodynamic limit and for $n \neq 1$ the chemical potential dependence on n associated with the ranges provided in Eq. (C1) of Appendix C being a smooth continuous function. On the one hand, as given in Eq. (B4), the ground state energies $E_{GS}(S_\eta - \delta S_\eta, -S_\eta + \delta S_\eta)$ and $E_{GS}(S_\eta, -S_\eta)$ have the same value. On the other hand, the non-LWS generated from the ground state of energy $E_{GS}(S_\eta, -S_\eta)$ have higher energy than that state. Therefore, for the Hamiltonian $\hat{H}$ of Eq. (B1) the energy eigenvalue $E(S_\eta, -S_\eta + n_\eta)$ with $n_\eta = \delta S_\eta$ of the energy eigenstate belonging to such a tower has the same number of electrons $N = N_a - 2S_\eta + 2n_\eta$ as the $n < 1$ ground states of η spin and η-spin projection $(S_\eta - \delta S_\eta)$ and $-(S_\eta - \delta S_\eta)$, respectively. The former state has larger energy than those ground states. Specifically, the following relation holds,

$$E(S_\eta, -S_\eta + n_\eta) = E_{GS}(S_\eta - n_\eta, -S_\eta + \delta S_\eta) + 2n_\eta|\mu|, \quad \delta S_\eta = n_\eta.\tag{B5}$$

Note that for $\delta S_\eta = n_\eta = 0$ the two energy eigenstates whose energies obey this relation are either the same state or two degenerate LWSs of the η-spin algebra. Since for $n_\eta > 0$ one has that $E_{GS}(S_\eta - \delta S_\eta, -S_\eta + \delta S_\eta) < E(S_\eta, -S_\eta + n_\eta)$, one finds full consistency with for $n < 1$ the ground state being a LWS of the η-spin algebra. Similar arguments confirm that $n > 1$ ground states are HWSs of the η-spin $SU(2)$ algebra.

Concerning the ground-state occupancies in terms of the objects or our operator representation, we note that the unitary transformation that relates electrons to rotated electrons preserves their number. Thus the number of rotated electrons equals that of electrons. Given that each one-site rotated-electron occupancy has two degrees of freedom, associated with the c hidden $U(1)$ symmetry and the ηs quasi-spin $SU(2)$ symmetry, respectively, the rotated-electron (and electron) numbers obey several exact relations. The following,

$$\begin{aligned} N_a - N &= M^{un}_{\eta,+1/2} - M^{un}_{\eta,-1/2} = M_{\eta,+1/2} - M_{\eta,-1/2}, \\ N_\uparrow - N_\downarrow &= M^{un}_{s,+1/2} - M^{un}_{s,-1/2} = M_{s,+1/2} - M_{s,-1/2}, \end{aligned}\tag{B6}$$

refer to the η-spin and spin degrees of freedom, respectively. Moreover, the relations,

$$\begin{aligned} N &= N_c + M^{bo}_\eta + 2M^{un}_{\eta,-1/2}, \\ &= M_s + M^{bo}_\eta + 2M^{un}_{\eta,-1/2}, \end{aligned}\tag{B7}$$

refer to the c hidden $U(1)$ symmetry and η-spin degrees of freedom and to the spin and η-spin degrees of freedom, respectively. The same applies to the following relations,

$$\begin{aligned} N^h &= N_c + M^{bo}_\eta + 2M^{un}_{\eta,+1/2}, \\ &= M_s + M^{bo}_\eta + 2M^{un}_{\eta,+1/2}, \end{aligned}\tag{B8}$$

where $N^h = (2N_a - N)$ is the number of holes. (Such holes are different from those associated with the hole concentration $x = (N_a - N)/N_a$. They are such that an unoccupied site has two holes, a singly occupied site has one hole, and one doubly occupied site has no holes.)

Above we have found that the η-spin $SU(2)$ algebra implies that $n \neq 1$ ground states are LWSs and HWSs of the η-spin algebra for $n < 1$ and $n > 1$, respectively. A $n = 1$ ground state is then both a LWS and HWS of that algebra. Furthermore, in Section V G it is confirmed that the η-spinons that are not invariant under the electron - rotated-electron unitary transformation have an anti-binding character. In the $N_a \to \infty$ limit the *minimum energy* for creation onto a $n \neq 1$ ground state of a η-spin singlet pair of anti-bound η-spinons is found in that section to

exactly equal that for creation onto it of a pair of unbound η-spinons of opposite η-spin projection. Relative to the zero-energy level of the Hamiltonian $\hat{H}$, Eq. (B1), the latter energy reads $(\varepsilon_{\eta,+1/2} + \varepsilon_{\eta,-1/2}) = 2|\mu|$ for $n \neq 1$, as given in Eq. (90). (The validity of the latter equation is confirmed below.) Such a zero-energy level coincides with that of the initial $n \neq 1$ ground state. Hence relative to it, creation of anti-bound η-spinons is a finite-energy process.

One then concludes that a $n < 1$ (and $n > 1$) ground state has no unbound $-1/2$ η-spinons (and no unbound $+1/2$ η-spinons) and no anti-bound η-spinons. The number of anti-bound η-spinons $M_{\eta}^{bo} = [N_a - 2S_c - 2S_{\eta}]$ given in Eq. (86) is, due to symmetry, always an integer even number. This is consistent with the corresponding η-spin-singlet configuration involving an equal number, $M_{\eta}^{bo}/2 = [N_a/2 - S_c - S_{\eta}]$, of η-spinons of η-spin projections $-1/2$ and $+1/2$, respectively. Hence the above ground-state vanishing occupancies may be rephrased in terms of general η-spinon occupancies (unbound and anti-bound) as follows: A $n < 1$ (and $n > 1$) ground state has no $-1/2$ η-spinons (and no $+1/2$ η-spinons). Indeed, both the energy for creation of one pair of unbound η-spinons of opposite η-spin projection and the minimum energy for creation of one η-spin-singlet pair of anti-bound η-spinons onto a $n < 1$ (and $n > 1$) ground state stem from the corresponding $-1/2$ η-spinon (and $+1/2$ η-spinon). This is consistent with a $-1/2$ η-spinon (and a $+1/2$ η-spinon) describing the η-spin degrees of freedom of a rotated-electron doubly occupied site (and rotated-electron unoccupied site), independently of it being a unbound or anti-bound η-spinon. Hence one may again rephrase the above ground-state vanishing occupancies as follows: A $n < 1$ (and $n > 1$) ground state has no rotated-electron doubly occupied sites (and no rotated-electron unoccupied sites).

One then finds by combining the above ground-state vanishing occupancies with the general exact relations of Eqs. (B6)-(B8) that a $m = 0$ and $n < 1$ (and $n > 1$) ground state of the $u > 0$ 1D Hubbard model has $N_c = 2S_c = N$ (and $N_c = 2S_c = N^h = [2N_a - N]$) c fermions, an equal number $M_s = N_c$ of spinons, $N_c^h = |N_a - N|$ c fermion holes, and an equal number $M_{\eta,+1/2} = M_{\eta} = 2S_{\eta} = N_a - N$ (and $M_{\eta,-1/2} = M_{\eta} = 2S_{\eta} = N - N_a$) of unbound $+1/2$ η-spinons (and unbound $-1/2$ η-spinons). This is consistent with a $m = 0$ and $n = 1$ ground state having no η-spinons and no c fermion holes and thus no rotated-electron doubly occupied and unoccupied sites. For such a ground state the c fermion momentum band is full.

Similar results are reached for finite spin densities, concerning the ground-state spin degrees of freedom. In the corresponding derivations, the energy scale $2\mu_B|H|$ plays the same role as $2|\mu|$ for the η-spin degrees of freedom. For instance, the spin $SU(2)$ symmetry algebra implies that $m \neq 0$ ground states are LWSs and HWSs of that algebra for $m > 0$ and $m < 0$, respectively. A $m = 0$ ground state is then both a LWS and HWS of the spin algebra. Hence for $m > 0$ (and $m < 0$) the ground state has no unbound $-1/2$ spinons (and no unbound $+1/2$ spinons) and at $m = 0$ it has no unbound spinons. The $s\nu$ fermions were shown in Section V G to involve binding spinon configurations, rather than anti-binding. From the interplay of this property with the spectra extracted from the exact BA solution, one then finds that ground states have no $s\nu$ fermions with $\nu > 1$ spinon pairs. On the other hand, except in the case of fully polarized states, they have a finite population of $s1$ fermions. For instance, for the electronic density range $n \in [0, 1]$, the spin degrees of freedom of a $m > 0$ (and $m < 0$) $u > 0$ ground state are described by $M_s = N$ spinons, $M_s^{bo} = 2N_{\downarrow}$ (and $M_s^{bo} = 2N_{\uparrow}$) bound spinons within $N_{s1} = N_{\downarrow}$ (and $N_{s1} = N_{\uparrow}$) $s1$ fermions, and $M_{s,+1/2} = N_{\uparrow} - N_{\downarrow}$ (and $M_{s,-1/2} = [N_{\downarrow} - N_{\uparrow}]$) unbound $+1/2$ spinons (and unbound $-1/2$ spinons).

Our above analysis confirms that for densities in the range $n \in [0, 1]$ and $m \in [0, n]$ the ground states are inside the BA solution subspace. After this has been confirmed, analysis of the BA solution spectra straightforwardly leads to the ground-state c and $s1$ band occupancies given in Section VI.

Next we derive the unbound η-spinon energies for $n \neq 1$. As a result of the η-spin $SU(2)$ symmetry of the Hamiltonian $\hat{H}_{symm}$, its ground-state energy $E_{GS}^0 = E_{GS}^0(S_{\eta})$ is the same for the LWS and HWS ground states for which $S_{\eta} = -S_{\eta}^{x3}$ and $S_{\eta} = S_{\eta}^{x3}$, respectively. Indeed for that Hamiltonian all $2S_{\eta}$ non-LWSs generated from a $S_{\eta} > 0$ ground state have the same energy. In contrast, the ground-state energy of the Hamiltonian $\hat{H}$ of Eq. (B1) depends both on the S_{η} and S_{η}^{x3} values, as given in Eq. (B2).

The continuous character for $N_a \to \infty$ and $n \neq 1$ of the chemical-potential curve $\mu = \mu(n)$ of Eq. (C1) of Appendix C implies that, except for terms of order $1/N_a$, the following relation between ground state energies of the Hamiltonian $\hat{H}$ provided in Eq. (B1) holds,

$$E_{GS}(S_{\eta} + 1/2, S_{\eta}^{x3} - \text{sgn}\{x\}1/2) = E_{GS}(S_{\eta}, S_{\eta}^{x3}), \quad x = (1 - n), \quad S_{\eta} > 0. \tag{B9}$$

On combining Eqs. (B2) and (B9) we confirm that,

$$\begin{aligned} \mu &= E_{GS}^0(S_{\eta} + 1/2) - E_{GS}^0(S_{\eta}) \geq 0, \quad x \in [-1, 0], \\ &= E_{GS}^0(S_{\eta}) - E_{GS}^0(S_{\eta} + 1/2) \leq 0, \quad x \in [0, 1]. \end{aligned} \tag{B10}$$

Indeed, when expressed in terms of the electron numbers rather than of the η-spin values, such relations are equivalent to the usual chemical-potential definition,

$$\mu = E_{GS}^0|_{N+1} - E_{GS}^0|_N. \tag{B11}$$

Furthermore, it follows from Eq. (C1) of Appendix C that the sign relation $\text{sgn}\{\mu\} = -\text{sgn}\{x\}$ where $x = (1-n)$ holds for $n \neq 1$, so that,

$$|\mu| = E_{GS}^0(S_\eta + 1/2) - E_{GS}^0(S_\eta), \quad S_\eta > 0, \quad n \neq 1. \tag{B12}$$

The relation $E_{GS}(S_\eta, -S_\eta) = E_{GS}(S_\eta - \delta S_\eta, -S_\eta + \delta S_\eta)$ given in Eq. (B4) for $\delta S_\eta < S_\eta$ between the energies of two $n < 1$ ground states reveals that creation or annihilation onto a $n < 1$ ground state of a finite number $M_{\eta,+1/2}^{un} = 2\delta S_\eta$ of unbound η-spinons of η-spin projection $+1/2$ is a vanishing-energy process. A similar relation $E_{GS}(S_\eta, S_\eta) = E_{GS}(S_\eta - \delta S_\eta, S_\eta - \delta S_\eta)$ between the energies of two $n > 1$ ground states where $\delta S_\eta < S_\eta$ confirms that creation or annihilation onto a $n > 1$ ground state of a finite number $M_{\eta,-1/2}^{un} = 2\delta S_\eta$ of unbound η-spinons of η-spin projection $-1/2$ is also a vanishing energy process.

On the other hand, a $n < 1$ (and $n > 1$) ground state state is a LWS (and HWS) of the η-spin algebra. Hence it has no η-spinons of η-spin projection $-1/2$ (and projection $+1/2$). A $n < 1$ ground state $|GS\rangle = |\Psi_{l_o, l_\triangle^0, u}\rangle$ of η-spin $S_\eta = -S_\eta^{x_3} = (x/2) N_a$ has $M_\eta^{un} = M_{\eta,+1/2}^{un} = 2S_\eta$ unbound η-spinons of η-spin projection $+1/2$. Those describe the η-spin $SU(2)$ symmetry degrees of freedom of a number $2S_\eta$ of rotated-electron unoccupied sites. The corresponding degrees of freedom of the c hidden $U(1)$ symmetry are described by an equal number $N_c^h = 2S_\eta$ of c fermion unoccupied sites.

We apply onto that $n < 1$ ground state the off-diagonal generator $\hat{S}_\eta^\dagger$ of the η-spin algebra given in Eq. (41). Such a process flips the η-spin projection of one unbound η-spinon. It transforms the ground state $|GS\rangle = |\Psi_{l_o, l_\triangle^0, u}\rangle$ onto an energy eigenstate $|\Psi_{l_o, l_\triangle, u}\rangle$ with one $-1/2$ unbound η-spinon, $n_\eta = M_{\eta,-1/2}^{un} = 1$. Within the occupancy configurations of that state, one rotated-electron unoccupied site has been replaced by a rotated-electron doubly occupied site. Such a process affects the rotated-electron site occupancy η-spin $SU(2)$ symmetry degrees of freedom. The corresponding degrees of freedom of the c hidden $U(1)$ symmetry are not affected. The number of c fermion unoccupied sites and thus of c fermion holes are preserved. There are neither changes in the spinon occupancy configurations associated with the spin $SU(2)$ symmetry degrees of freedom. Analysis of the corresponding BA solution energy spectra, confirms that no energy contributions arise from the c fermions and spinons, whose occupancy configurations remain unchanged.

Furthermore, by the well known properties of the η-spin $SU(2)$ symmetry algebra, for the Hamiltonian $\hat{H}_{symm}$ of Eq. (2) such a rotation in the η-spin space does not change the energy. Hence $\langle\Psi_{l_o, l_\triangle^0, u}|\hat{H}_{symm}|\Psi_{l_o, l_\triangle^0, u}\rangle = \langle\Psi_{l_o, l_\triangle, u}|\hat{H}_{symm}|\Psi_{l_o, l_\triangle, u}\rangle$ where the energy $\langle\Psi_{l_o, l_\triangle^0, u}|\hat{H}_{symm}|\Psi_{l_o, l_\triangle^0, u}\rangle$ is that of the initial ground state, $|GS\rangle = |\Psi_{l_o, l_\triangle^0, u}\rangle$. The operator $\hat{S}_\eta^\dagger$ commutes with the electron - rotated-electron unitary operator. Thus such a process enhances the number of both electrons and rotated-electrons by two. From the use of Eq. (B3) one then finds,

$$\langle\Psi_{l_o, l_\triangle, u}|\hat{H}|\Psi_{l_o, l_\triangle, u}\rangle = \langle\Psi_{l_o, l_\triangle, u}|\hat{H}_{symm}|\Psi_{l_o, l_\triangle, u}\rangle - 2\mu = \langle\Psi_{l_o, l_\triangle, u}|\hat{H}_{symm}|\Psi_{l_o, l_\triangle, u}\rangle + 2|\mu|, \quad n < 1. \tag{B13}$$

In the above process, one unbound $+1/2$ η-spinon is annihilated and one unbound $-1/2$ η-spinon created. We have shown above that annihilation and creation of one unbound $+1/2$ η-spinon is a zero-energy process for an initial $n < 1$ ground state. Hence it follows from Eq. (B13) that relative to that ground state, creation onto it of the unbound η-spinon of η-spin projection $-1/2$ and corresponding rotated-electron doubly occupied site is a process of energy $2|\mu|$.

If instead one applies the η-spin algebra generator $\hat{S}_\eta$ of Eq. (41) onto a $n > 1$ ground state $|GS\rangle = |\Psi_{l_o, l_\triangle^0, u}\rangle$ of η-spinon $S_\eta = S_\eta^{x_3} = (-x/2) N_a$ and thus $M_\eta^{un} = M_{\eta,-1/2} = 2S_\eta$ unbound η-spinons of η-spin projection $-1/2$, one finds similar results. Specifically, we find that relative to such a ground state, creation onto it of the unbound $+1/2$ η-spinon and corresponding rotated-electron unoccupied site is a process of energy $2|\mu|$. One then concludes that the energy $\varepsilon_{\eta,\pm1/2}$ for creation onto a $n \neq 1$ ground state of one unbound η-spinon of η-spin projection $\pm1/2$ is given by Eq. (87). Our analysis focused on the η-spin $SU(2)$ symmetry algebra. A similar analysis involving the spin $SU(2)$ symmetry algebra leads to the unbound spinon energy provided in Eq. (89).

Finally, we derive the $n = 1$ unbound η-spinon energies from analysis of the energy spectrum associated with creation and annihilation of one electron onto and from the $n = 1$ and $S_\eta = 0$ ground state, respectively. The η-spin rotations considered above generate changes in $S_\eta^{x_3}$ that are restricted to integer values. In turn, the transitions between ground states whose electron numbers differ by one considered here are associated with half integer $\pm1/2$ deviations in $S_\eta^{x_3}$. The well-defined discontinuity at $n = 1$ in the chemical-potential curve $\mu = \mu(n)$, Eq. (C1) of Appendix C, reveals that the energy eigenvalues of the Hamiltonian of Eq. (B1) two ground states with numbers $S_\eta = 0, S_\eta^{x_3} = 0$ and $1/2, -\text{sgn}\{x\}1/2$, respectively, are related as follows,

$$E_{GS}(1/2, \mp1/2) = E_{GS}(0,0) + (\mu^0 \pm \mu), \quad S_\eta = 0, \quad \mu \in [-\mu^0, \mu^0]. \tag{B14}$$

Here μ^0 is the one-electron gap and $2\mu^0$ the corresponding Mott-Hubbard gap given in Eqs. (C3) and (C4) of Appendix C.

The transitions between ground states whose electron numbers differ by one affect all three degrees of freedom, associated with c hidden $U(1)$ symmetry and two $SU(2)$ symmetries. Creation of one electron onto such a ground state involves annihilation of one c fermion, annihilation of one spinon, and creation of one $-1/2$ η-spinon. On the other hand, annihilation of one electron from a $n = 1$ ground state involves annihilation of one c fermion, annihilation of one spinon, and creation of one $+1/2$ η-spinon.

For simplicity, we consider initial ground states of zero spin density, $m = 0$. The final unbound η-spin energy expressions are the same at $m = 0$ and for finite m. Only the energy scales μ and μ^0 in such expressions have m dependent values. The unbound η-spin energies considered here are relative to the zero-energy level of the Hamiltonian $\hat{H}$, Eq. (B1). (Due to symmetry, relative to that of the Hamiltonian $\hat{H}_{symm}$ of Eq. (2) such energies vanish.) The use of the exact BA solution reveals that the above annihilation of one c fermion and one spinon involved in the ground-state - ground-state one-electron excitations considered here are in the thermodynamic limit and relative to the zero-energy level of the Hamiltonian $\hat{H}$ of Eq. (B1) zero-energy processes. It then follows that that Hamiltonian energy eigenvalues deviations under such one-electron addition and removal excitations correspond to the energy for creation of the $-1/2$ η-spinon and $+1/2$ η-spinon, respectively.

We consider two types of excitations. (i) Addition of removal or one electron. And (ii) addition or removal of one electron plus one η-spin rotation. The latter rotation has as initial state a η-spin $1/2$ ground state. It is populated by a single unbound η-spinon of η-spin projection $+1/2$ or $-1/2$. The η-spin rotation flips it to $-1/2$ or $+1/2$, respectively. In the derivation of the energy spectra of the two types of excitations relative to the zero-energy level of the Hamiltonian $\hat{H}$ of Eq. (B1) the ground-state-energy relation of Eq. (B14) is used. One then readily finds that relative to the zero-energy level of that Hamiltonian the energy for creation onto a $n = 1$ ground state of one unbound $\pm 1/2$ η-spinon is that given in Eq. (88). Finally, the relations given in Eqs. (90) and (91) follow directly from the expressions provided in Eqs. (87)-(89).

Appendix C: Useful energy scales

In this Appendix we introduce several energy scales that are extracted from the BA solution and play an important role in the studies of this paper.

The chemical potential curve $\mu = \mu(n)$ and magnetic energy scale $2\mu_B H = 2\mu_B H(m)$ associated with the magnetization curve are defined in Eq. (163). The corresponding chemical-potential dependence on the hole concentration $x = (1 - n)$ is such that,

$$\mu(x) = -\mu(-x); \quad \mu(x) \in [\mu^0, \mu^1], \quad x \in [-1, 0]; \quad \mu \in [-\mu^0, \mu^0], \quad x = 0,$$
$$\mp\mu^1 = \lim_{x \to \pm 1} \mu(x); \quad \mp\mu^0 = \lim_{x \to 0^\pm} \mu(x); \quad \mu^1 > \mu^0. \tag{C1}$$

The finiteness for $u > 0$ of the one-electron gap, μ^0, implies that the chemical potential curve $\mu = \mu(x)$ has a well-defined discontinuity at $n = 1$. For $u \gg 1$ and $m = 0$ the chemical potential curve is such that the energy scale $2\mu = 2\mu(x)$ is of the form,

$$2\mu(x) = -\text{sgn}\{x\}[U - 4t \cos(\pi x)], \quad x \in [-1, 0] \text{ and } x \in [0, 1],$$
$$\in [-(U - 4t), (U - 4t)], \quad x = 0. \tag{C2}$$

For $u > 0$ and $n = 1$ the Mott-Hubbard gap remains finite for all spin densities $m \in (-1, 1)$. It is an even function of m. For instance, at $m = 0$ and $m = -1, 1$ it is given by [2],

$$2\mu^0 = U - 4t + 8t \int_0^\infty d\omega \frac{J_1(\omega)}{\omega (1 + e^{\omega \, 2u})} = \frac{16 \, t^2}{U} \int_1^\infty d\omega \frac{\sqrt{\omega^2 - 1}}{\sinh\left(\frac{2\pi t \omega}{U}\right)}, \quad m = 0,$$
$$= \sqrt{(4t)^2 + U^2} - 4t, \quad m = -1, 1, \tag{C3}$$

respectively, where $J_1(\omega)$ is a Bessel function. For $u \ll 1$ and $u \gg 1$, this energy scale behaves as,

$$2\mu^0 \approx \frac{8}{\pi}\sqrt{t\,U}\, e^{-2\pi\left(\frac{t}{U}\right)}, \quad m = 0; \quad 2\mu^0 \approx \frac{U^2}{8t}, \quad m = -1, 1, \quad u \ll 1,$$
$$2\mu^0 \approx [U - 4t], \quad m \in [-1, 1], \quad u \gg 1. \tag{C4}$$

The energy scale $2\mu^1$ associated with the minimum $-\mu^1$ and maximum μ^1 chemical-potencial values is for all m magnitudes given by,

$$2\mu^1 = [U + 4t]. \tag{C5}$$

On the other hand, the magnetic energy scale $2\mu_B H$ in Eq. (163) dependence on the spin density m is such that,

$$
\begin{aligned}
2\mu_B H(m) &= -2\mu_B H(-m)\,; \quad 2\mu_B H(m) \in (0, 2\mu_B H_c)\,, \quad m \in (-[1-|x|], 0)\,, \\
2\mu_B H(0) &= 0\,; \quad \mp 2\mu_B H_c = \lim_{x \to \pm[1-|x|]} 2\mu_B H(m)\,, \quad x = (1-n)\,.
\end{aligned}
$$
(C6)

A closed-form expression for the dependence on U, t, and density n of the energy scale $2\mu_B H_c$ associated with the critical field H_c can be derived from the general $2\mu_B H$ expression provided in Eq. (163) [59]. Since $2\mu_B H_c$ is a even function of the hole concentration $x = (1-n)$, we expressed it in terms of it,

$$
\begin{aligned}
2\mu_B H_c &= \frac{1}{2}\sqrt{(4t)^2 + U^2}\left[1 + \frac{2}{\pi}\operatorname{arccot}\left(\frac{\sqrt{(4t)^2 + U^2}}{U}\tan(\pi|x|)\right)\right] \\
&\quad - U(1 - |x|) + \frac{4t}{\pi}\cos(\pi x)\arctan\left(\frac{4t\sin(\pi|x|)}{U}\right)\,, \quad x = (1-n)\,.
\end{aligned}
$$
(C7)

At $u = 0$ and for $u \gg 1$ its limiting behaviors are,

$$
\begin{aligned}
2\mu_B H_c &= 4t\sin^2\left(\frac{\pi x}{2}\right)\,, \quad u = 0\,, \quad x = (1-n)\,, \\
&= \frac{8(1 - |x|)t^2}{U}\left[1 + \frac{\sin(2\pi|x|)}{2\pi(1 - |x|)}\right]\,, \quad u \gg 1\,, \quad x = (1-n)\,.
\end{aligned}
$$
(C8)

As a function of n, it has for instance the following values,

$$
\begin{aligned}
2\mu_B H_c &= 0\,, \quad n = 0, 2\,, \\
&= \frac{1}{2}\left[\sqrt{(4t)^2 + U^2} - U\right]\,, \quad n = \frac{1}{2}, \frac{3}{2}\,, \\
&= \sqrt{(4t)^2 + U^2} - U\,, \quad n = 1\,.
\end{aligned}
$$
(C9)

Other energy scales involved in our studies are the c and $\alpha\nu$ fermion energy dispersions given in Eqs. (161) and (162). Both the momentum widths $2\pi(1-n)$ and $2\pi m$ of the $\eta\nu$ and $s\nu \neq s1$ momentum bands, respectively, and their energy-dispersion bandwidths, $[\varepsilon_{\alpha\nu}^0(q_{\alpha\nu}) - \varepsilon_{\alpha\nu}^0(0)]$, where $\alpha\nu = \eta\nu$ and $\alpha\nu = s\nu \neq s1$, vanish in the $n \to 1\,; m \to 0$ limit. Hence for the $n = 1$ and $m = 0$ ground state the corresponding $\alpha\nu \neq s1$ fermion energy dispersions defined in Eqs. (161) and (162) do not exist. On the other hand, the c fermion energy dispersions $\varepsilon_c^0(q)$ and $\varepsilon_c(q)$ and $s1$ fermion energy dispersions $\varepsilon_{s1}^0(q)$ and $\varepsilon_{s1}(q)$ have closed-form expressions, which read,

$$
\begin{aligned}
\varepsilon_c^0(q) &= -\frac{U}{2} - 2t\cos k_c^0(q) - 4t\int_0^\infty d\omega \frac{\cos(\omega\,\sin k_c^0(q))}{\omega(1 + e^{\omega U/2t})} J_1(\omega)\,, \quad q \in [-\pi, \pi]\,, \\
\varepsilon_c(q) &= \varepsilon_c^0(q) + \mu^0\,, \quad q \in [-\pi, \pi]\,, \\
\varepsilon_{s1}(q) &= \varepsilon_{s1}^0(q) = -2t\int_0^\infty d\omega \frac{\cos(\omega\,\Lambda_{s1}^0(q))}{\omega\,\cosh(\omega u)} J_1(\omega)\,, \quad q \in [-\pi/2, \pi/2]\,.
\end{aligned}
$$
(C10)

In this equation, $J_1(\omega)$ is a Bessel function and the $n = 1$ and $m = 0$ ground-state rapidity functions $k_c^0(q)$ (such that $\Lambda_c^0(q) = \sin k_c^0(q)$) and $\Lambda_{s1}^0(q)$ are defined in terms of their inverse functions as follows,

$$
\begin{aligned}
q &= k_c^0(q) + 2\int_0^\infty d\omega \frac{\sin(\omega\,\sin k_c^0(q))}{\omega(1 + e^{2\omega u})} J_0(\omega)\,, \quad q \in [-\pi, \pi]\,, \\
q &= \int_0^\infty d\omega \frac{\sin(\omega\,\Lambda_{s1}^0(q))}{\omega\,\cosh(\omega u)} J_0(\omega)\,, \quad q \in [-\pi/2, \pi/2]\,.
\end{aligned}
$$
(C11)

Here $J_0(\omega)$ is again a Bessel function.

On the other hand, for $m \to 0$ and $n \in [0, 1]$ all $s\nu \neq s1$ bands momentum and energy bandwidths vanish. For a $m = 0$ ground state the corresponding $s\nu \neq s1$ fermion energy dispersions defined by Eqs. (161) and (162) do not exist. For densities $n \in [0, 1]$ and $m = 0$ the c fermion, $s1$ fermion, and $\eta\nu$ fermion energy dispersions $\varepsilon_c(q)$, $\varepsilon_{s1}(q)$,

and $\varepsilon_{\eta\nu}^0(q)$, respectively, defined in such equations have the following limiting behaviors for $u \to 0$ and $u \gg 1$,

$$
\begin{aligned}
\varepsilon_c(q) &= -4t \left[\cos\left(\frac{q}{2}\right) - \cos\left(\frac{\pi n}{2}\right) \right], \quad |q| \leq 2k_F = \pi n, \quad u \to 0, \\
&= -2t \left[\cos\left(|q| - \frac{\pi n}{2}\right) - \cos\left(\frac{\pi n}{2}\right) \right], \quad 2k_F = \pi n \leq |q| \leq \pi, \quad u \to 0, \\
&= -2t \left[\cos(q) - \cos(\pi n) \right] \\
&\quad - \frac{8 n t^2}{U} \ln(2) \left[\sin^2(q) - \sin^2(\pi n) \right], \quad |q| \leq \pi, \quad u \gg 1,
\end{aligned}
\tag{C12}
$$

$$
\begin{aligned}
\varepsilon_{s1}(q) &= \varepsilon_{s1}^0(q) = -2t \left[\cos(q) - \cos\left(\frac{\pi n}{2}\right) \right], \quad |q| \leq k_F = \pi n/2, \quad u \to 0, \\
&= -\frac{2\pi n t^2}{U} \left[1 - \frac{\sin(2\pi n)}{2\pi n} \right] \cos\left(\frac{q}{n}\right), \quad |q| \leq k_F = \pi n/2, \quad u \gg 1,
\end{aligned}
\tag{C13}
$$

$$
\begin{aligned}
\varepsilon_{\eta\nu}^0(q) &= 4t \cos\left(\frac{|q| + \pi n}{2}\right), \quad |q| \leq (\pi - 2k_F) = \pi (1 - n), \quad u \to 0, \\
&= \frac{8t^2(1 - n)}{\nu U} \left[1 - \frac{\sin(2\pi(1 - n))}{2\pi (1 - n)} \right] \cos^2\left(\frac{q}{2(1 - n)}\right), \quad |q| \leq (\pi - 2k_F) = \pi (1 - n), \quad u \gg 1.
\end{aligned}
\tag{C14}
$$

Also in the limit of an initial fully polarized ground state corresponding for instance to $m \to n$ for electronic densities $n \in [0, 1]$, the energy dispersions $\varepsilon_c^0(q)$ and $\varepsilon_c(q)$, $\varepsilon_{s\nu}^0(q)$ and $\varepsilon_{s\nu}(q)$, and $\varepsilon_{\eta\nu}^0(q)$ and $\varepsilon_{\eta\nu}(q)$ defined by Eqs. (161) and (162) have closed-form expressions,

$$
\begin{aligned}
\varepsilon_c^0(q) &= -\frac{U}{2} - 2t \cos q, \quad q \in [-\pi, \pi], \\
\varepsilon_c(q) &= -2t[\cos q - \cos(\pi n)], \quad q \in [-\pi, \pi], \\
\varepsilon_{s\nu}^0(q) &= -\frac{2t}{\pi} \int_{-\pi n}^{\pi n} dk \sin k \arctan\left(\frac{[\sin k - \Lambda_{s\nu}^0(q)]}{\nu u}\right), \quad q \in (-2k_F, 2k_F) = (-\pi n, \pi n), \\
\varepsilon_{s\nu}(q) &= \varepsilon_{s\nu}^0(q) + W_{s\nu}, \quad q \in (-2k_F, 2k_F) = (-\pi n, \pi n), \\
\varepsilon_{\eta\nu}^0(q) &= -\nu U + 4t \mathrm{Re}\left[\sqrt{1 - (\Lambda_{\eta\nu}^0(q_j) + i\nu u)^2}\right] \\
&\quad - \frac{2t}{\pi} \int_{-\pi n}^{\pi n} dk \sin k \arctan\left(\frac{[\sin k - \Lambda_{\eta\nu}^0(q)]}{\nu u}\right), \quad q \in (-[\pi - 2k_F], [\pi - 2k_F]) = (-\pi[1 - n], \pi[1 - n]), \\
\varepsilon_{\eta\nu}(q) &= \varepsilon_{\eta\nu}^0(q) + W_{\eta\nu}, \quad q \in (-[\pi - 2k_F], [\pi - 2k_F]) = (-\pi[1 - n], \pi[1 - n]).
\end{aligned}
\tag{C15}
$$

In this limit one has that $k_c^0(q) = q$, whereas the rapidity functions $\Lambda_{\alpha\nu}^0(q)$ appearing in the above expressions are defined by their inversion functions,

$$
\begin{aligned}
q &= 2\mathrm{Re}[\arcsin(\Lambda_{\eta\nu}^0(q_j) + i\nu u)] \\
&\quad + \frac{1}{\pi} \int_{-\pi n}^{\pi n} dk \arctan\left(\frac{[\sin k - \Lambda_{\eta\nu}^0(q)]}{\nu u}\right), \quad q \in (-[\pi - 2k_F], [\pi - 2k_F]) = (-\pi[1 - n], \pi[1 - n]), \\
q &= -\frac{1}{\pi} \int_{-\pi n}^{\pi n} dk \arctan\left(\frac{[\sin k - \Lambda_{s\nu}^0(q)]}{\nu u}\right), \quad q \in (-2k_F, 2k_F) = (-\pi n, \pi n).
\end{aligned}
\tag{C16}
$$

Moreover, for the electronic density range $n \in [0, 1]$ and spin density $m \to n$ the $s\nu$ and $\eta\nu$ energy dispersion bandwidths of Eq. (164) appearing in some of the expressions provided in Eq. (C15) are given by,

$$
\begin{aligned}
W_{s\nu} &= \frac{1}{2}\sqrt{(4t)^2 + (\nu U)^2} \left[1 - \frac{2}{\pi} \mathrm{arccot}\left(\frac{\sqrt{(4t)^2 + (\nu U)^2}}{(\nu U)} \tan(\pi n)\right) \right] \\
&\quad - \nu U n - \frac{4t}{\pi} \cos(\pi n) \arctan\left(\frac{4t \sin(\pi n)}{\nu U}\right), \quad n \in [0, 1], \quad m \to n,
\end{aligned}
\tag{C17}
$$

and

$$W_{\eta\nu} = \frac{1}{2}\sqrt{(4t)^2 + (\nu U)^2}\left[1 + \frac{2}{\pi}\operatorname{arccot}\left(\frac{\sqrt{(4t)^2 + (\nu U)^2}}{(\nu U)}\tan(\pi n)\right)\right]$$
$$- \nu U\,(1 - n) + \frac{4t}{\pi}\cos(\pi n)\arctan\left(\frac{4t\sin(\pi n)}{\nu U}\right)\,,\quad n \in [0,1]\,,\quad m \to n\,, \tag{C18}$$

respectively. The energy bandwidths $W_{s\nu}$ and $W_{\eta\nu}$ given here are an increasing and decreasing function of n, respectively. For instance, for $n \to 0$, $n = 1/2$, and $n = 1$ they read,

$$\begin{aligned} W_{s\nu} &= 0\,,\quad n \to 0\,,\quad m \to n\,, \\ &= \frac{1}{2}\left[\sqrt{(4t)^2 + (\nu U)^2} - U\right]\,,\quad n = \frac{1}{2}\,,\quad m \to n\,, \\ &= \sqrt{(4t)^2 + (\nu U)^2} - \nu U\,,\quad n = 1\,,\quad m \to n\,, \end{aligned} \tag{C19}$$

and

$$\begin{aligned} W_{\eta\nu} &= \sqrt{(4t)^2 + (\nu U)^2} - \nu U\,,\quad n \to 0\,,\quad m \to n\,, \\ &= \frac{1}{2}\left[\sqrt{(4t)^2 + (\nu U)^2} - U\right]\,,\quad n = \frac{1}{2}\,,\quad m \to n\,, \\ &= 0\,,\quad n = 1\,,\quad m \to n\,, \end{aligned} \tag{C20}$$

respectively.

For spin density $m = 0$ and electronic density $n = 1$ all energy bandwidths $W_{\alpha\nu}$ vanish except that of the $s1$ fermion energy dispersion, which reads,

$$W_{s1} = 2t\int_0^\infty d\omega\,\frac{J_1(\omega)}{\omega\,\cosh(\omega\,u)}\,,\quad n = 1\,,\quad m = 0\,. \tag{C21}$$

Finally, for $u \to 0$ and $u \gg 1$, electronic densities $n \in [0,1]$, and spin densities $m = 0$ and $m \to n$ the $s\nu$ and $\eta\nu$ dispersion energy bandwidths of Eq. (164) have the following limiting behaviors,

$$\begin{aligned} W_{s\nu} &= \delta_{\nu,1}\left\{2t\left[1 - \cos\left(\frac{\pi}{2}n\right)\right]\right\}\,,\quad m = 0\,,\quad u \to 0\,, \\ &= 4t\sin^2\left(\frac{\pi n}{2}\right) = 2\mu_B\,H_c\,,\quad m \to n\,,\quad u \to 0\,, \\ &= \delta_{\nu,1}\left\{\frac{2\pi n\,t^2}{U}\left[1 - \frac{\sin(2\pi n)}{2\pi n}\right]\right\} = \delta_{\nu,1}\frac{\pi}{4}\left(2\mu_B\,H_c\right)\,,\quad m = 0\,,\quad u \gg 1\,, \\ &= \frac{8n\,t^2}{\nu U}\left[1 - \frac{\sin(2\pi n)}{2\pi n}\right] = \frac{1}{\nu}\,2\mu_B\,H_c\,,\quad m \to n\,,\quad u \gg 1\,, \end{aligned} \tag{C22}$$

and

$$\begin{aligned} W_{\eta\nu} &= 4t\cos\left(\frac{\pi}{2}n\right) = 2|\mu|\,,\quad m = 0\,,\quad u \to 0\,, \\ &= 4t\left[1 - \sin^2\left(\frac{\pi n}{2}\right)\right] = 2|\mu|\,,\quad m \to n\,,\quad u \to 0\,, \\ &= \frac{8(1 - n)\,t^2}{\nu U}\left[1 - \frac{\sin(2\pi(1 - n))}{2\pi(1 - n)}\right]\,,\quad m = 0\,,\quad u \gg 1\,, \\ &= \frac{8n\,t^2}{\nu U}\frac{\sin(2\pi\,n)}{2\pi\,n}\,,\quad m \to n\,,\quad u \gg 1\,, \end{aligned} \tag{C23}$$

respectively.

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